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Effective Parameters of Hydrogeological Models

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ISSN 2191-5369 e-ISSN 2191-5377
ISBN 978-3-642-23721-8 e-ISBN 978-3-642-23722-5
DOI 10.1007/978-3-642-23722-5
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2011940202

Cover design: eStudio Calamar, Berlin/Figueres

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Dedicated to my wife
Inna Gorokhovskaia
and to the memory of our son
Iaroslav Gorokhovski
(1963–2011)

Preface

This book concerns the uncertainty of the hydrogeological modeling. In a sense, it is a development of the ideas published long ago (Gorokhovski 1977). The topic of that book was impossibility of evaluating the uncertainty of the simulation results in a provable quantitative way. The book happened to be a success: I had difficulty finding its copies for my friends, some prominent hydrogeologists and geological engineers started treating me with more respect, and some colleagues stopped speaking to me for a long time. But no other consequences followed.

I personally was not fully satisfied. The book was mostly a critique based on common sense and illustrated by simple and transparent examples from hydrogeology and geological engineering. The examples could be easily verified, using just a calculator. The book stated that the impossibility to evaluate the uncertainty of simulation results does not preclude obtaining the results which are best in a reasonably defined sense, though the uncertainty of those best results remains unknown. But I had a vague notion of how to assure such results at that time.

Quantitative predictions of responses of geological objects on man made and natural impacts were, are, and will remain in the foreseeable future a considerable element of engineering design and decision making. Even at that time and even in the Soviet Union, where I resided and worked, it was possible to simulate many applied hydrogeological processes, though access to the pertinent software and computers was not easy, at least for me (see Afterword for more details). At present, due to the fast development of computers and numerical methods, we can simulate almost any process based on contemporary concepts and theories. The gravest obstacle remains uncertainty of the simulation results caused by paucity of the available data on properties of geological objects, boundary conditions, and impacts when the natural impacts are affecting factors. So, one of the main issues, in my opinion, is how to assure that the yielded results are the best, and effective in the sense best is defined. I hope that this book is a considerable step to yielding the effective simulation results.

The uncertainty of the results of hydrogeological modeling was and is discussed intensively. Thus, Beck (1987) writes: “The difficulties of mathematical modeling are not questions of whether the equations can be solved and the cost of solving them many times; not are they essentially questions of whether priory theories (on transport, dispersion, growth, decay, predation, etc.) is potentially capable of describing the system's behavior. The important questions are those whether the priory theory adequately matches observed behavior and whether the predictions obtained from models are meaningful and useful." Oreskes et al. (1994), hold that geological models "predictive value is always open to question." (See also Oreskes 2003, 2004). This is not surprising, since in hydrogeology "the modeling assumptions are generally false and known to be false" (Morton 1993, Beven 2005). I could continue this list of quotations. But let me restrict myself with one more. As Beven (2004), puts it mildly: "There is uncertainty about uncertainty." I think he is wrong: the uncertainty of the hydrogeological modeling is the fact about which there is no uncertainty. Indeed: "It's a fundamental tenet of philosophy of science that the truth of a model can never be proved; only disproved", (Mesterton-Gibbons 1989).

The above quotations are a tribute to academism really. Experienced hydrogeologists are well aware of the uncertainty of most of their conclusions. And the reason is obvious. The models include properties and combinations of the properties of geological objects. Those must be known continuously, at least, when differential or integral equations are involved. That is, they must be known at each point of the object and at each instant of the simulation period, excluding sets of isolated points and instants. But geological objects are inaccessible to direct observations and measurements and the data on them are sparse. The geological models are a tool to interpolate and extrapolate the sparse data at every point of the geological object which they represent in simulations and at every instant of the periods of the simulations. The tool is limited. The geological interpolation and extrapolation are based on the principle that geological settings of the same origin, composition, and geological history have the same properties. This principle leads to so-called piecewise homogeneous geological models. Sometimes the properties are subjected to spatial trends whose mathematical descriptions are arbitrary in essence (Chap. 3). So how can we evaluate in a quantitative way the reliability of the geological models with respect to a problem at hand? It suffices just common sense to conclude that it is impossible except, maybe, in some rare cases.

Since the issue is not simulations, solving the corresponding equations, but the uncertainty of the yielded results, the question arises, what to do? US EPA (1987), gives the answer related to environmental predictions, including hydrogeological ones: "It should be recognized that the data base will always be inadequate, and eventually there will be a finite sum that is dictated by time, common sense, and budgetary constraints. One simply has to do the best one can with what is available". Unfortunately, US EPA (1987), does not explain what is and how 'to do the best'.

The situation seems to be clear enough: it is impossible to evaluate the uncertainty of simulation results of the hydrogeological models in a provable quantitative way. But, contrary to its own statement cited above (US EPA, 1989), holds that "Sensitivity and uncertainty analysis of environmental models and their predictions should be performed to provide decision-makers with an understanding of the level of confidence in model results and to identify key areas for future study". It claims also that "A number of methods have been developed in recent years for quantifying and interpreting the sensitivity and uncertainty of models". NCR (1990), states "Over the past decade, the development of stochastic modeling techniques has been useful in quantitatively establishing the extent to which uncertainty in model input translates into uncertainty in model prediction." Binley and Beven (1992), Beven and Freer (2001) and Beven (2005) suggest a general likelihood framework for uncertainty analysis, recognizing that it includes some subjective elements and, therefore, in my opinion, may not be provable. Hill et al. (2000) suggest the algorithm and program, permitting evaluating the uncertainty of simulation results. Cooley (2004) suggests a theory for making predictions and estimating their uncertainty. And so on (Feyen and Caers 2006; Hassan and Bekhit 2008; Rojas et al. 2008, 2010; Ch and Mathur 2010; Mathon et al. 2010; Ni et al. 2010; Singh et al. 2010a, b; Zhang et al. 2009; and many others).

Although the number of publications providing the methods as if quantifying uncertainty of the results hydrogeological modeling growths very fast, the philosophical tenet mentioned above leaves us still with the only real option: "to do the best one can with what is available". In this book, it means obtaining the best simulation results in the sense of the least squares criterion on a given monitoring network, though other criteria of the efficiency are also possible. Besides, the required best must relate not to the best fit during model identifications (calibrations), but to the best results in the coupled predictive simulations. Such simulation results are called effective. To achieve the predictive efficiency for a given simulation model, we need to find the effective parameters, that is, the parameters making the pertinent predicting or evaluating effective. A model furnished with the effective parameters is called effective. Once more, the goal must be the models which are effective in predictive simulations and extended evaluations, and not in model identification procedures like calibration. This can be achieved by introducing the transforming mechanisms converting the actual properties of geological bodies into effective parameters of the predictive models (Chap. 5). Chapters 6 and 7 contain examples of such mechanisms. The standard procedure for evaluating the transforming mechanisms is called by me the two-level modeling (Chap. 8). The transforming mechanisms can be applied for solving inverse problems (Chap. 9). The notion of the inverse problem in this book differs from the standard one accepted in hydrogeological modeling. That is, the inverse problem is understood as evaluating properties of more complex models using less complex ones. Chapter 10 is a short conclusion. I included in the book Chap. 11 also where I compare my Soviet and American experiences as a teacher and a scientist. I hope it may by interesting for readers.

I hope that this book is helpful for modelers working with the underground flows and mass transport. But its main addressees are common hydrogeologists and, maybe, students of hydrogeology and environmental sciences. I knew and know many excellent hydrogeologists who never differentiated or integrated anything after passing the final tests on calculus. For these reasons, I resort to the sound sense and the simplest mathematical models and examples, rather of the conceptual nature, i.e., “constructed to elucidate delicate and difficult points of a theory” (Lin and Segel 1974, Kac 1969) as much as I can. However, the approach to alleviating the issue of the uncertainty of the results of hydrogeological simulations suggested in this book requires intensive computational calculations. This does not permit avoiding mathematics completely. But the mathematics applied in the text is mostly the least squares method. The examples and the results are transparent and easy to understand and to interpret even for those readers who do not want to mess with mathematics.

Acknowledgements This book would not be possible without help of many people from different walks. Among them I have to mention first experienced hydrogeologist and dear friend L.S. Jazvin, who passed away recently. Our uncompromised disputes have done a lot to form my approaches to hydrogeological modeling. Fair criticism and support of my friends and colleagues, B.V. Borevsky, M.T. Oyzerman, M.V. Rats, and V.V. Trofimov helped me in the development of the two-level modeling approach. I cannot but mention V.I. Sedletsky without whom the probability of my coming to the United States and writing this book had been extremely low. This book would be impossible without Dr. Zia Hosseinipour who found a project for me in this country and helped, as well as our dear friends Mr. and Mrs. Donald and Karen Goodel, to get and to settle me and my wife here. I thank and value my American supervisors, Drs. James Martin, Donald Nute, Dan Kannon and Jim Weaver who became my friends. They were kind to let me apply my strange approaches to the problems they assigned to me. I thank my sons Vikenti and Iaroslav for their support and help. And of course, this endeavor would be impossible without support, help and endurance of my beloved wife Inna.

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Abstract

Effective Parameters of Hydrogeological Models Geological models applied in predictive hydrogeological modeling are not exact replicas of the objects they represent. Manifold of details related to structures and properties of the objects remains unknown. Those details affect the simulation results considerably, differently and unpredictably for different formulations of the simulation problem. They cause the phenomenon of problem-dependence of model identification and make the model parameters effective in calibration ineffective in predictive simulations. Due to them the provable evaluation of uncertainty of the simulation results is impossible. However this does not preclude obtaining the best, effective, simulation results based on the available data and predefined criteria of quality of predicting. To provide such results, transforming mechanisms are introduced. They are mathematical expressions for evaluating the model parameters which are effective in predictive simulations. Examples of the mechanisms are provided as well as a method for their evaluations. Shown also how the mechanisms can be used for interpretation hydrogeological data which is possible due to the mention above phenomenon of the problem-dependence. In his last chapter author compares the conditions under which he worked in the Soviet Union (35 years) and in the United States (20 years) which may be interesting for readers.

Chapter 1
Introduction

Although hydrogeological conditions can be of interest per se, most hydrogeological investigations are of applied nature, and their results are used in decision-making that may carry large ecological and financial risks. For example, when developing a reservoir project, the developers have to evaluate possible losses of water from the reservoir, the stability of the dam, and how adjacent soils and rocks could be affected by different project decisions. Hydrogeological investigations related to the use of an aquifer for water supply should not only conclude that the usage is possible. The developers must also have estimates on how long and with what intensity the aquifer can be exploited by a well or group of wells. The developers of a landfill project must know whether the landfill can cause contamination of the aquifer below and, if so, whether and when the contaminant plume will reach water supply wells and the concentration of the pollutant at the wells. The developers of an irrigation project need to know to what extent and how fast the water table rise should be expected, what consequences are possible, how to deal with them effectively, etc.

The point is that, for projects that affect the geological surroundings to be effective environmentally and economically, the responses of the surroundings to the planning impacts must be taken into consideration. To this end, the goal of applied hydrogeological investigations is to provide quantitative predictions of those responses. Moreover, to make a correct or optimal decision, decision-makers must know the errors of the quantitative predictions. (The term “to predict” relates to processes developing in time. In this text it is used also as a synonym for the term “to evaluate” in cases of evaluating some instant value or steady-state conditions, if such usage does not cause confusion).

The usual tool for obtaining quantitative hydrogeological predictions is mathematical modeling, i.e., solving differential and integral equations describing the pertinent processes or states. The mathematical models are applied to geological models substituting for real geological objects. In this book, the mathematical models are assumed to be adequate, i.e., that they reproduce the processes of

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_1,

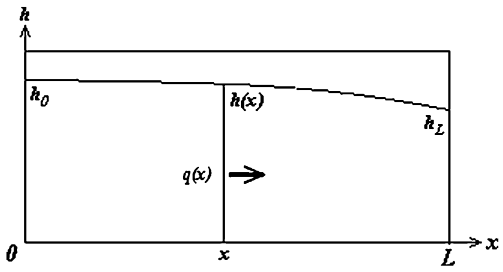

Fig. 1.1 One-dimensional steady-state flow on the interval [0, *L*]

interest sufficiently accurately. This is not true in general, but mathematical models recognized by the professional community and applied properly usually yield satisfactory approximations of reality (see Sect. 4.4). The main source of error occurring in simulations is the distinction between predictive geological models and actual geological objects, and inaccurate or often just wrong boundary conditions, though inaccuracies of the mathematical models also contribute to those errors. Since the geological surroundings are inaccessible to direct observations and measurements, and data on them are sparse, the issue is how the parts of geological objects which are unknown or wrongly represented by geological models can affect the accuracy of the simulation results.

Let us start with a simple example: steady-state filtration in an unconfined aquifer on a horizontal base when recharge is absent (Fig. 1.1). Under the Dupuit–Forchheimer assumption, considering the vertical component of the Darcy velocity to be negligibly small, the filtration can be treated as one dimensional. It is governed by the following ordinary differential equation:

$$\frac{\mathrm{d}\left(K(x)h(x)\frac{\mathrm{d}h}{\mathrm{d}x}\right)}{\mathrm{d}x} = 0, \tag{1.1}$$

where $h(x)$ is the thickness of the aquifer at point x and $K(x)$ is the hydraulic conductivity varying along the x-axis. Equation 1.1 is derived based on the law of conservation and the Darcy law stating that the velocity of filtration q (the Darcy velocity, specific flux) is equal to

$$q = -K(x)\frac{\mathrm{d}h}{\mathrm{d}x}. \tag{1.2}$$

The boundary conditions are the thickness of the aquifer at the ends of the interval [0, L], which is assumed to be known: $h(0) = h_0$ and $h(L) = h_L$.

Let the goal be to evaluate the thickness of the aquifer at any arbitrary location x within the interval [0, L]. To this end, we have to integrate Eq. 1.1. Its first integration yields

$$2K(x)h(x)\frac{\mathrm{d}h}{\mathrm{d}x} = C,$$

where C is an arbitrary constant (the factor of 2 being used to simplify Eq. 1.3 below). Assuming that $K(x) \neq 0$ in the interval [0, L], we can rewrite the above equation as

$$2h(x)\mathrm{d}h = C\frac{\mathrm{d}x}{K(x)}.$$

Integrating the above equation, we obtain

$$2\int_0^x h(x)\mathrm{d}h = h^2(x) - h^2(0) = C\int_0^x \frac{\mathrm{d}x}{K(x)}. \tag{1.3}$$

To obtain a unique solution to Eq. 1.1, we need to define the arbitrary constant C. To this end we use the second boundary condition at $x = L$:

$$h_L^2 = C\int_0^L \frac{\mathrm{d}x}{K(x)} + h_0^2 \text{ and } C = -\frac{h_0^2 - h_L^2}{\int_0^L \frac{\mathrm{d}x}{K(x)}}.$$

Then, the solution to Eq. 1.1 with the given boundary conditions takes the form

$$h^2(x) = h_0^2 - \left(h_0^2 - h_L^2\right)\frac{\int_0^x \frac{\mathrm{d}x}{K(x)}}{\int_0^L \frac{\mathrm{d}x}{K(x)}}. \tag{1.4}$$

Thus, to obtain the thickness of the aquifer, $h(x)$, at an arbitrary point x within the interval [0, L], we need to know the boundary conditions h_0 and h_L at the ends of the interval and the hydraulic conductivity, $K(x)$, continuously, i.e. at each point of the interval, excluding perhaps a countable set of points (i.e., a set of points that can be enumerated, meaning separated from each other).

However, knowing $K(x)$ at each point of the interval of interest is not possible physically or economically. A few, sparse measurements of the hydraulic conductivity are available at best. We need to fill in the information gap by interpolating and extrapolating the available data on the hydraulic conductivity over all points of the interval [0, L]. Tools for doing this are geological (structural) models (which I prefer to call geological ones, to emphasize that geologists with their knowledge of geological settings and their spatial variability play the most important role in interpolating and extrapolating geological data). The tools are usually limited and even primitive. They are based on the principle that soils and rocks of the same origin, lithological composition, geological age, and history are homogeneous geologically; that is, each property of a geologically homogeneous structure is considered constant. Simple trends in the property values are permissible, if the data reveal some spatial tendencies. Model calibration is also a tool for generalization of the variable property values of interest in the predictive model parameters (see Chap. 4). Another approach to filling the information gap is the use of random functions as a tool for describing spatial distributions of the geological properties (see Chap. 3). Both approaches can be combined: geologists assign boundaries of geologically homogeneous parts of a site, and different regressions and random functions can be used within those geologically homogeneous parts.

The simplest interpolation in the considered example is recognizing the aquifer as homogeneous within the interval [0, L] with constant hydraulic conductivity $K(x) = \hat{K}$. Then, the constant hydraulic conductivity $\hat{K}$ can be factored out from Eq. 1.1 or 1.4 and canceled, converting Eq. 1.4 into

$$h^2(x) = h_0^2 - \left(h_0^2 - h_L^2\right)\frac{x}{L}. \tag{1.5}$$

So, as soon as the homogeneous model of the aquifer is chosen, the predicted aquifer thickness does not depend on the hydraulic conductivity at all. Since the actual hydraulic conductivity is not constant, the simulation results will carry errors. The only possible estimate for these errors is that the real water table elevations are between h_0 and h_L. The errors are equal to zero at the ends of the interval [0, L] and reach the maximal absolute value somewhere inside the interval. The magnitude of the error does not exceed $|h_0 - h_L|$.

Let the previous scheme (Fig. 1.1) represent a cross-section of a channel and a capturing drain, and the goal be to evaluate the losses, flux Q, from the channel to the drain parallel to the channel. The geological model is still homogeneous, though the geological object is not. The losses depend on the hydraulic conductivity of the rocks and soils between the channel and the drain. Assuming the steady-state regime and absence of infiltration within the interval [0, L], we obtain the constant flux Q which is described by the following equation at arbitrary point x within the interval [0, L]:

$$Q = -K(x)h(x)\frac{\mathrm{d}h}{\mathrm{d}x}. \tag{1.6}$$

Separating variables, we can rewrite Eq. 1.6 as

$$Q\frac{\mathrm{d}x}{K(x)} = -h(x)\mathrm{d}h. \tag{1.7}$$

Integrating Eq. 1.7 with the same boundary conditions [$h_0 = h(0)$ and $h_L = h(L)$] yields

$$Q = -\frac{h_0^2 - h_L^2}{2\int\limits_0^L \frac{\mathrm{d}x}{K(x)}}. \tag{1.8}$$

In the case of the homogeneous model, Eq. 1.8 yields

$$\hat{Q} = -\hat{K}\frac{h_0^2 - h_L^2}{2L}. \tag{1.9}$$

So, to evaluate the losses Q accurately, the effective hydraulic conductivity $\hat{K}$ of the homogeneous model must be assigned as

$$\frac{1}{\hat{K}} = \frac{1}{L}\int_0^L \frac{\mathrm{d}x}{K(x)}. \tag{1.10}$$

If the acceptable losses Q are known, and the soil between the canal and the drain can be compacted, Eq. 1.9 could be applied to evaluate the necessary degree of compression of the soil, but this is not the point here. Contrary to the case of evaluating the thickness of the aquifer, applying the homogeneous model, in this case we are not able to evaluate the upper boundary for errors of the predicted losses Q, if we do not know the range of the actual values of the hydraulic conductivities $K(x)$. However, Eq. 1.10 gives the rule for assigning the hydraulic conductivity to the homogeneous models to evaluate the errors, considering the Dupuit–Forchheimer assumption to be acceptable. It should be the *weighted harmonic mean* of the actual hydraulic conductivities.

The most popular geological models represent geological sites as consisting of homogeneous subintervals such that, within subinterval $[x_{i\text{-}1}, x_i]$, the hydraulic conductivity is constant and equal to K_i. Then Eq. 1.10 can be rewritten as

$$\frac{1}{\hat{K}} = \frac{1}{L}\sum_{i=1}^{n}\left(\frac{1}{K_\mathrm{i}}\int_{x_{\mathrm{i}-1}}^{x_\mathrm{i}} \mathrm{d}x\right) = \frac{1}{L}\sum_{i=1}^{n}\frac{\Delta x_\mathrm{i}}{K_\mathrm{i}}, \tag{1.11}$$

where n is the number of homogeneous subintervals and $\Delta x_i = x_i - x_{i-1}$. Thus, the hydraulic conductivity of the homogeneous model must be assigned as the harmonic mean weighted with respect to the length of the homogeneous subintervals. If the errors ΔK_i for the hydraulic conductivities K_i within each subinterval $[x_i, x_{i\text{-}1}]$ are known, evaluating the errors of the model parameter $\hat{K}$ and the flux Q becomes possible.

The above examples demonstrate that not only the geological settings, but also the formulation of the simulation problem, define the choice of model parameters. Thus, when evaluating the thickness of the aquifer on the horizontal aquitard by applying a homogeneous model under the Dupuit–Forchheimer simplification, we do not need to worry about choosing the model hydraulic conductivity at all (rather avoid the homogeneous model in such sorts of problems). However, when evaluating the flux, we do need to do this. Moreover, as demonstrated in Chap. 6, the effective hydraulic conductivities (the model characteristics providing the best fit of the simulation results to the observations) depend on the monitoring network. As shown in Chap. 7, the effective hydraulic transmissivities can depend on time also.

Gomez-Hernandez and Gorelick (1989) hold that, “if there is no best effective hydraulic conductivity …, the predictive capability of the model must be questioned.” Why? The two examples above illustrate the well-known phenomenon called the problem dependence of model identification (Gorokhovski 1977; Carrera and Neuman 1986; Yeh 1986; Kool et al. 1987; Hornung 1990; van Genuchten et al. 1990; Bear et al. 1992). The phenomenon does affect the predictive capability of the models. This means that the effective parameters of a predictive model may be different for different formulations of the simulation problem. Namely, the issue of obtaining model parameters that are effective in predictive simulations, not just in calibrations, is the main point of this book.

Let us consider two simple examples of assigning the hydraulic conductivity values to our homogeneous model according to Eq. 1.10 [more examples can be found in Gorokhovski (1977)]. In these examples, functions $K(x)$ are such that integral 1.10 can be found in any textbook on integral calculus.

First, let the hydraulic conductivity be a linear function of the coordinates: $K(x) = \frac{K_L - K_0}{L} x + K_0$,
where $K_0 = K(0)$ and $K_L = K(L)$. Then, according to Eq. 1.10,

$$\frac{1}{\hat{K}} = \frac{1}{L} \int_0^L \frac{\mathrm{d}x}{\frac{K_L - K_0}{L} x + K_0} = \frac{1}{K_L - K_0} \ln \frac{K_L}{K_0}.$$

Thus,

$$\hat{K} = \frac{K_L - K_0}{\ln \frac{K_L}{K_0}}. \tag{1.12}$$

Second, let the hydraulic conductivity be an exponential function:

$$K(x) = K_0 \mathrm{e}^{-\frac{x}{L}}.$$

Substituting the above $K(x)$ into Eq. 1.10, we obtain

$$\frac{1}{\hat{K}} = \frac{1}{L} \int_0^L \frac{\mathrm{d}x}{K_0 \mathrm{e}^{-\frac{x}{L}}} = \frac{1}{K_0} \int_0^L \mathrm{e}^{\frac{x}{L}} \frac{\mathrm{d}x}{L} = \frac{1}{K_0} (\mathrm{e} - 1).$$

So in this case

$$\hat{K} = \frac{K_0}{\mathrm{e} - 1}. \tag{1.13}$$

Equations 1.12 and 1.13 also represent the harmonic means of the actual values of hydraulic conductivities under their specific spatial distributions. What is important is that no statistical or probabilistic concepts or notions are applied to yield these results; they have been obtained based on the usual deterministic approach. Equation 1.11 is, for example, a complete analogy to the well-known rule for calculating the total resistance of series electrical circuits. The horizontal filtration along layers with fixed hydraulic heads at the ends of the interval of interest in a confined aquifer is analogous to an electrical parallel circuit. So, the hydraulic conductivity for evaluating the flux when applying a homogeneous model must be the *arithmetic mean* of the hydraulic conductivity of the layers, weighted by their thicknesses.

There exist many ways for estimating the errors of a function caused by errors in its parameters. Let a model be represented by the function

$$y = f(x, P), \tag{1.14}$$

where x is an independent variable or a vector (list) of independent variables and $P = (P_1, P_2, \ldots, P_i, \ldots, P_n)$ is a vector (list) of the governing parameters. Then, the errors of the model Δy caused by the errors of the parameters ΔP can be estimated, for example, as

$$|\Delta y| \le \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f(x,P)}{\partial P_i} \Delta P_i \right)^2}$$

or

$$|\Delta y| \le \sum_{i=1}^{n} \left| \frac{\partial f(x,P)}{\partial P_i} \Delta P_i \right|. \tag{1.15}$$

Estimates (1.15) are provable only if Eq. 1.14 represents the phenomenon of interest adequately. If not all the parameters affecting the modeled phenomenon are not included in the list P, then it can happen that Estimates (1.15) are still acceptable, if we are lucky, but the obtained errors are not provable.

If we had complete information on a geological object but for some reason were going to simulate its response on an impact, using simplified geological models, we could, at least in principal, evaluate the errors resulting from the simplification. However, if we simplify something that we do not know in full, we cannot evaluate the consequences of our simplifications. This is where, in my opinion, the central issue of hydrogeological modeling lies. Computer power at present is such that we are able to make predictions based on the highest theoretical level of the hydrogeological sciences (Beven 1989). However, there is a gap between the data necessary for making predictions and the available pertinent data. We do not know the accuracy of the function $K(x)$ which we use in our simulations. Applying a piecewise homogeneous model, we may miss some homogeneous parts of the real site or add inexistent ones. We almost never know the exact locations of boundaries between the homogeneous parts, and so on. We fill such informational gaps with assumptions. However, “the modeling assumptions are generally false and known to be false” (Morton 1993; Beven 2005). Consequently, we cannot obtain provable estimated errors of the simulation result.

The use of false or unprovable assumptions does not make the results necessary wrong. They may be acceptable practically. For example, the Dupuit–Forchheimer simplification neglecting the vertical component of the Darcy velocity in all our previous examples is wrong and contradictory. However, as Muskat (1946) observed, the resulting fluxes "will nevertheless be surprisingly close to those given empirically or by exact calculations." False or untested assumptions do not permit provable estimation of errors and the uncertainty of the simulation results, which are important for informed decision-making. However, they do not preclude achieving the best result or making the best decisions in some circumstances.

Two approaches to hydrogeological modeling exist at present. I call one of them engineering and the other geostatistical. The first approach is based on practical engineering experience. The second one is based on statistical methods which are developed to work with incomplete and erroneous data. The approaches do not exclude each other: the engineering approach includes some statistical features, and the geostatistical one essentially uses the elements of the engineering approach. Unfortunately, neither of them provides provable estimates of the simulation result uncertainty, as discussed in detail in Chaps. 2 and 3.

"To do the best" (US EPA 1987), we need first to define "the best" reasonably, keeping our expectations in line with our possibilities. For example, we can request that our estimation be the best one in the sense of the least-squares method on a given monitoring network; or, which model and its parameters are the best in a given situation may be the subjective opinion of an expert based on his or her experience. After we define the meaning of "the best," we need to furnish our model (models) with the set (sets) of values of the model parameters providing the best prediction in the defined sense. We are not able to evaluate the uncertainty of our best decision yet. However, what we can do is to make our decisions more informed. There is not one way to this end, and a concept for one such approach, based on transforming mechanisms and two-level modeling, is suggested in this book (Chaps. 5–9).

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Chapter 2
Engineering Approach

In 1992, the journal *Advances in Water Resources* published a series of papers on validation of hydrogeological models. In one of those papers, Konikow and Bredehoeft (1992) hold that groundwater models cannot be validated but only invalidated. This means that the real quality of a model can be judged only by comparing the prediction produced by the model with what actually occurred, only based on post audit, and that accurate results in the process of model calibration do not warrant that the model will predict accurately. However, if calibration goes wrong, the model cannot be trusted. Commenting on their paper, De Marsily et al. (1992) write:

> We all know that the parameters of a model are uncertain, probably wrong in many cases, and easily can be invalidated. Similarly, the 'structures' of the model (2-D, multi-layered, 3-D, etc.) can be incorrectly chosen. So what? As long as they reproduce the observed behavior of the system, we can use them to make predictions. It also seems to us that the better or the longer the reproduction of the observed behavior, the more confident we can be of their validity. … Using the model in a predictive mode and comparing it with new data is not a futile exercise; it makes a lot of sense to us. It does not prove that the model will be correct for all circumstances; it only increases our confidence in its value. We do not want certainty; we will be satisfied with engineering confidence.

Writing this chapter, I had a strong urge to call it "So What?" and to use as an epigraph the last sentence of the above quotation. However, I overcame this urge and named it instead after the engineering approach. It is simple and conceptually transparent. Indeed, the modeling assumptions are generally "false and known to be false" (Morton 1993; Beven 2005). However, working on many similar projects in similar geological surroundings and observing the results of implementation of those projects, professionals gain personal and collective experience of what models work satisfactorily, how their parameters and boundary conditions should be assigned to yield satisfactory results, and the chance that a given model will fail, which is a factual, empirical estimate of the uncertainty of the simulation results. Validated in such a probabilistic way, a model can be considered as a

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_2,

"sound, fulfilling all necessary conditions, and just good enough model" (McCombie and McKinley 1993).

Let us come back to the models based on the Dupuit-Forchheimer assumption, i.e., that when the gradient of a water table is small enough, the vertical component of the Dupuit velocity can be neglected and the flow considered as strictly horizontal. Such simplifications are fairly common in mathematical physics or engineering. Muskat (1946) calls the Dupuit-Forchheimer assumption "not trustworthy." However, he expresses his astonishment at the fact that the results of its application are accurate compared with "those given empirically or by exact calculations." Haitjema (1995) holds that "a Dupuit-Forchheimer model could have done the job, saving resources and cost." Since the Dupuit-Forchheimer assumption is false, there is no possibility to evaluate the errors of simulation results based on it in a closed way, i.e., based on errors of the model structure and its parameters. However, Beven (1981) considers it reasonable for water table slopes that are mild, and according to Bear (1972), it generates practically acceptable errors for a homogeneous shallow aquifer on a horizontal aquitard, if the squared slope of the water table is less then 0.01.

Such use of unprovable and even wrong assumptions (let us call them simplifications), which lead to accepted practical results under some empirically established conditions, I call the engineering approach. My attitude with respect to this approach is rather positive. It recognizes the reality of the impossibility of evaluating the uncertainty of predictions in a provable way. I would rather trust the professionals, though I understand that their experience is subjective and that this is different from an objective proof. However, this trust, though cautious, relates to situations where the engineering approach really exists, e.g., in the case of building small reservoirs, or drilling water supply wells for small farms or family houses. However, what does one have to do if there is no such experience, e.g., when a project is unique per se, or unique for a given surroundings? Or what does one have to do if experienced professionals make different recommendations and estimations?

Lerner (1985) described several cases related to groundwater supply in Africa, Latin America, and England in which teams of highly qualified experts made different but equally incorrect estimations and predictions, using the same data. Anderson and Woessner (1992) report several instances with unencouraging results of post audit in the USA. They explain the failures by errors in conceptual models in developing which the professional experience plays the major role. Andersen and Lu (2003) add several more examples of post audits that "have not provided high confidence in the predictive accuracy" of the applied models.

In relatively good times for Soviet hydrogeology, an extensive study of the reliability of hydrogeological estimates of groundwater resources was undertaken (Yazvin 1972). The study of 89 large intakes from artesian aquifers revealed that only in 12 cases was the accuracy of the predictions satisfactory. The resources were considerably underestimated in 76 cases and overestimated in 1 case. The study of 25 intakes from alluvial aquifers revealed that the resources were considerably overestimated in 20 cases. In all 114 cases the estimates of groundwater resources were approved by the Central Commission on Ground Water Resources of the USSR, consisting of highly experienced hydrogeologists. In most of the above examples, professional expertise was combined with model calibration, and this fact aggravates the situation even more.

It may be consoling, at least in part, that other fields where completeness of geological information is essential share the same plight. One of the most well-documented examples demonstrating that the uncertainty of geological modeling is not just an abstract issue is the complete failure of geophysical data interpretation relating to superdeep drilling at Kola Peninsula, Russia (Kola 1984) and in Bavaria, Germany (Kerr 1993). As drilling revealed, actual geological structures differed completely from those anticipated. The same happened for the superdeep bore in Azerbaijan (Kola 1984). These failures cannot be explained by the scarcity of data or unsatisfactory ability of the interpretational teams. In such expensive enterprises as superdeep drilling, the teams certainly were the best, and the data (with respect to their amount and quality) exceeded what is available in routine enterprises. The failures were caused by the use of the "sound, fulfilling all necessary conditions, and just good enough," but nevertheless fallible, models recognized by the professional communities. Bredehoeft (2005) calls this "the conceptualization model problem" and gives several examples from his and his colleagues' hydrogeological practice in the USA. Problems, including civilian and economical, related to uncertainty of predictions made by experts in seismology are discussed by Geschwind (1997), Hanks (1997), and many others. Unfortunately, professionalism and credentials do not always warrant confidence in models and simulation results.

The viewpoint that engineering confidence is good enough to trust predictions is usually grounded on two groups of arguments. First, during their studies and professional activity, practitioners accumulate knowledge and develop thorough professional experience on where and how geological and mathematical models should be applied to yield practically meaningful results. We have discussed this kind of arguments above.

The second is that all human progress is founded on the use of invalidated or even provably incorrect models. Indeed, it is true that "astronomers, on the basis of a few days of observations, will predict asteroid and comet orbits for thousands of years with good accuracy" (McCombie and McKinley 1993). Their argument can be even strengthened by mentioning one of the greatest achievements of those models: Le Verrier's discovery "on pen's point" of Neptune based on peculiarities of Uraniums' orbit. He calculated the orbit of the unknown planet, and Neptune was discovered exactly at the location he predicted.

Somehow, it is less well known that Le Verrier explained in the same way the peculiarities of Mercury's orbit (Levy 1973). This hypothesis was never confirmed. Its failure gave birth to several other hypotheses that failed also. It is recognized at present that Einstein's theory of relativity explains Mercury's behavior. My point is that there has never once been a need to revise astronomic models.

Effective modern technologies based on models that are impossible to validate can be included in this argument also. However, each such technology undergoes extensive testing, and then, when it is applied, e.g., in manufacturing new products, special attention is paid to controlling the quality of raw materials, to assembly, and to other pertinent procedures. Final products are also tested. For example, each airplane and ship undergoes thorough tests.

In hydrogeology we do not have such luxuries. Each hydrogeological site is unique. We cannot control its geological structure or even know the structure in full. Its response is also unique and depends on impacts. The impacts can be intensive and diverse, and many of them do not have analogs in the past. We do not have long enough periods of observations, and no prediction for a period of more than a 100 years has actually been tested. In science, if a hypothesis is proved to be wrong, another hypothesis takes its place, then another, and another, etc. In hydrogeology, it may be too late to seek another model when it becomes clear that the applied one is faulty.

Professionalism is a necessary condition for obtaining meaningful results, especially for the development of geological models. As Tsang (1992) points out, a sick person should go to an expert having an MD degree. However, faith in professional judgment as always true is also a fallacy.

Finally, let me repeat. If a professional has experience obtained on many similar projects in similar environments and has observed the results of implementation of those projects, it could be reasonable to trust in the professional's judgment. Often such professionals do not need any mathematical modeling, they just know what works (In Athens, Georgia, where I am typing these lines, I have never seen geological engineering or geotechnical explorations supporting projects for developing residential middle-class neighborhoods. The builders just know what kind of foundations must be used). However, in the case of projects which are very expensive and carry large environmental and financial risks, it is difficult if not impossible to find a professional with the pertinent experience. Even if such a professional exists, it is not reasonable to rely on his or her subjective opinion. We need models (quantitative theories) to predict what can happen, and of course we need professionals for developing conceptual geological models. However, if the professional's judgment about the uncertainty related to the use of some model in some situation is supported by pertinent statistics, it should be taken into consideration. When such statistics is not available, nothing can be said about the quality or the uncertainty of the results obtained in the framework of the engineering approach.

However, contemporary computational techniques and methods permit the development of a surrogate for engineering experience. This surrogate cannot provide provable estimates of uncertainty either. However, it permits more informed decision-making (see Chaps. 5–10).

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Chapter 3
Geostatistical Approach

The situation with the deterministic approach to predictive simulations is transparent. It can provide evaluations of the uncertainty of the simulation results in some typical circumstances for which engineering experience exists. These evaluations are of statistical nature. They are based on observed successes and failures of decisions made based on results of the corresponding simulations. However, if such experience does not exist, the engineering approach fails to provide provable estimates for the uncertainty of the simulation results. The situation seems more complicated with the geostatistical approach.

Statistics is the science which deals with incompletely known and fallible data, which makes it so appealing to hydrogeologists (Shvidler 1963, 1964; Dagan 1986; Graham and McLaughlin 1989; Gomez-Hernandez and Gorelick 1989; NRC 1990; Review 1990; Cooley 2004; and many others). Thus, van Genuchten et al. (1990) write "Because measurements and model predictions are both subject to uncertainty, the parameter estimation problem is essentially a statistical problem." More than this, geostatistics has come with the promise to quantify the uncertainty of hydrogeological simulations: "…geostatistics has been integrated with hydrogeology to provide methods for quantifying uncertainty where estimation, interpolation, and extrapolation of hydrogeologic attributes are required between and beyond data locations" (Kitandis 1997).

This widespread notion that statistics is a sufficient tool to overcome paucity of geological data and provide provable estimates for the uncertainty of simulation results is a fallacy; geostatistical estimates are strongly conditioned by many assumptions. As demonstrated below, some of those assumptions are impossible to test, and some are known to be invalid. This means that the accuracy of geostatistically acquired results cannot be proven. In this sense, the deterministic and geostatistical approaches do not differ. Moreover, the geostatistical approach makes use of all or nearly all the assumptions of the deterministic one, plus many others. This alone makes it more vulnerable. Thus, averaging processes popular in geostatistical applications and resulting in the harmonic, geometric, or arithmetic

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_3,

means of actual hydraulic conductivity and transmissivity values are not related to the probability distributions of these properties. They emerge from deterministic formulations of some filtration problems, as shown in Chap. 1. When a specific averaging process is defined (deterministically) and the probability distributions of the pertinent properties are known, then we can use statistical methods to estimate the errors of those deterministically inferred parameters and the simulation results. So, if we reject the deterministic approach, the geostatistical estimates do not make sense. However, if we accept it, we can still doubt its geostatistical extensions, if they are based on unverified or knowingly false assumptions.

Even if the statistical assumptions are valid, the geostatistical approach may be irrelevant. Thus, real groundwater flows always depend on the hydraulic conductivity and its variability. However, simulated hydraulic heads are not affected by the hydraulic conductivity; if the geological model is homogeneous, filtration is steady state and governed by the Laplace equation with prescribed hydraulic heads as boundary conditions (Eq. 1.5). This shows that the geostatistical formulations of some real problems can be meaningless. Therefore, before applying them, we must demonstrate their relevance to the problem at hand. Mentioning the paucity and inaccuracy of the pertinent information is insufficient. It is the same situation as with numerical algorithms: not every algorithm is unstable, but because unstable algorithms exist, we must demonstrate each time that the algorithm which we apply is stable when applied to the given problem.

It must be noted that the proponents of geostatistics understand the artificial nature of the introduction of geostatistics into hydrogeology. Thus, Review (1990) holds: "It should be noted here that the decision to select random functions to model a regionalized variable is only a matter of analytical convenience. This does not imply that the phenomenon under study is indeed random." Indeed, the hydraulic conductivity $K(x)$ in the problem leading to Eq. 1.1, reproduced here for convenience,

$$\frac{\mathrm{d}\left(K(x)h(x)\frac{\mathrm{d}h(x)}{\mathrm{d}x}\right)}{\mathrm{d}x} = 0,$$

is unique for a given site and is not a random function. The fact that the measured values of $K(x)$ carry random errors does not make $K(x)$ a random function either. We can try to minimize the errors resulting in estimation of the thickness $h(x)$ of the aquifer or of flux Q. To this end we can use, say, a regression equation approximating $K(x)$ by a least squares regression applied to available measurements of the hydraulic conductivity. In so doing, we are still in the frame of the deterministic approach. However, when we assume that $K(x)$ is a random function, we assume that what we observe within our site is only one realization of the function $K(x)$. Since we have only one, deterministic distribution of the hydraulic conductivity, the following question arises: Where are the others? They must belong to other, analogous, sites. So, we assume that our site is an element of an ensemble comprising many sites. The goal becomes to find the stochastic characteristics of that ensemble and than apply them to our one. To solve this additional problem, we have to resort to a number of additional assumptions that can be as convenient and as false as the assumption that $K(x)$ is a random function.

Now let us assume that we have finally solved our problem; we got some result, which may be practically acceptable. Can we prove that our estimate of the uncertainty of our result is true? We can, if all our assumptions are true, but not if even just one of them is false or untested. So, let us consider some geostatistical assumptions and practice in more detail.

3.1 Ensembles

The concept of an ensemble is fundamental to the geostatistical approach (Dagan 1986). Conclusions, statements, and results of the statistical approach are related to ensembles or to their elements with respect to ensembles: We estimate expected values of properties and other statistics for an ensemble, the property's correlation and autocorrelation functions within the ensemble, the probability of a quantity characterizing an element to be within some range of the ensemble values of the same nature, etc. To evaluate an element belonging to an ensemble means to place it within the ensemble. To this end, we must know the statistical properties of the ensemble. If they are not known, but many other elements of the ensemble are available, we can try to use the available elements and statistical methods to evaluate the ensemble properties and then proceed with the element of interest. However, in geostatistical applications to hydrogeology, the site we have to work with is only one available element of an unknown ensemble. It is unique, and it is not obvious where to look for and find the others. To overcome this conceptual difficulty, or rather to forget it, geostatisticians suggest that "the ensemble does not actually exist" (Dagan 1986).

The statistical approach does not make much sense if there is no ensemble. So, we need to make up the ensemble, one element of which is our site. Since the unknown ensemble "is only a matter of analytical convenience," making it up is not an issue. Following Dagan (1986), we assume that the made-up ensemble is stationary (ergodic). This permits one to ascribe to the made-up ensemble the statistical properties of the "random" functions observed at our site. Note that, even if an observed function exhibits some kind of stationarity within our site, the statement about stationarity of the made-up ensemble is still just a hypothesis which is impossible to test, since only one element (one realization of the pertinent random functions) is available.

Thus, the site of interest, the only available element of the made-up ensemble, is assigned to be the mathematical expectation (the mean) of the made-up ensemble. The flow within the site becomes the mean flow for the made-up ensemble, and all geostatistical characteristics of the made-up ensemble can be estimated based on the available observations on our site. In this way, we obtain, or rather make up, all necessary geostatistical data and can proceed to evaluate the uncertainty of the results of our predictive problem.

Unfortunately, for the reasons discussed in Sect. 3.5 and Chap. 4 and well known to geostatisticians, the use of the mean characteristics of an ensemble does not warrant the mean response of the ensemble on a given impact. However, let us forget about this for a while and ask the following question: How probable is it that the only sample from an ensemble coincides with the ensemble's mean? The answer is obvious: not very. However, does this question make sense? For our convenience, we constructed our made-up ensemble in such a way that this should happen for sure.

However, what does one have to do, if a property, e.g., the hydraulic conductivity as a function of coordinates, is not obviously stationary? No problem again: Dagan (1986) suggests generalizing the definition of stationarity, "allowing for instance for polynomial trends and stationary increments."

The polynomial trend is the universal and most convenient tool for describing regional trends besides, maybe, Fourier decomposition. We can try polynomials of different order until we find a polynomial that satisfies our taste. The only limitation is the maximal order of the polynomial, which depends on the number of available observations. The polynomial of maximal possible order, though very attractive since its residuals equal zero, is not stable with respect to additional data.

In general, the mathematical description of a trend is a compromise between fulfilling the following requirements:

1. Reasonable considerations about the geological structure of the site.
2. Simplicity depending on the amount of data available and the intended application of the trend description.
3. Minimization of the sum of the squared residuals.

The first two of these requirements are obviously subjective. The third follows from the first two. Thus, our judgment about the mathematical description of regional trends and even their existence are hypotheses that are impossible to prove. They may be more realistic than our hypotheses related to the random functions and the made-up ensemble, but still remain hypotheses.

Figure 3.1 illustrates the possibility of polynomial trend descriptions (data from Bondarik 1974). Only polynomials of 1st, 2nd, 7th, and 14th orders are presented in Fig. 3.1. The polynomial of 14th order is not stable, and the goodness-of-fitness criterion is not defined for it. Instead, we could use linear interpolation between neighboring observations. However, then our regional trend becomes nondifferentiable at points of observation. Polynomial trends have the advantage of being differentiable everywhere.

So we can use 15 polynomials, including the polynomial of zeroth order, that is, the mean value of the observations, and many other mathematical representations to describe the regional trend and, according to Dagan (1986), convert our made-up ensemble into a stationary one. However, can we prove that our choice is correct? Even if some of the polynomials can be practically close within the region of interest, the situation remains the same: just the number of alternatives

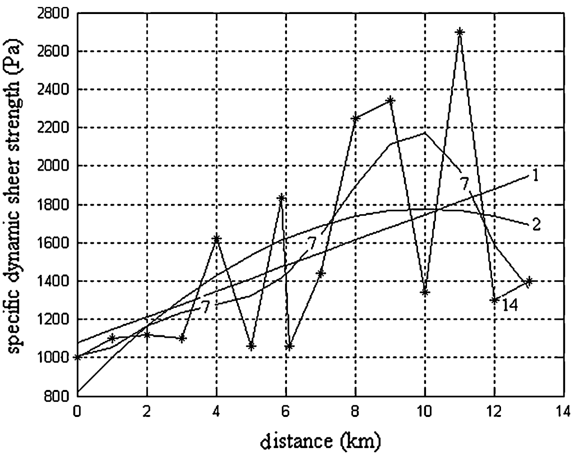

Fig. 3.1 Polynomial trends based on the same factual data represented by stars

decreases slightly. However, we would be extremely lucky if the true trend were present in our set of alternatives. Note also that, if we need derivatives of the regionalized variable, we should understand that different representations of the trend can lead to essentially different derivatives.

I do not know about you, but I feel some discomfort, since the made-up ensemble remains arbitrary. It seems that Dagan feels the same. So, he recommends "to check a posteriori whether the stationary assumptions are met at a given degree of significance" and to use "some prior information derived from similar sites" (Dagan 1986).

I understand his first recommendation as testing the statistical homogeneity of the residuals. I doubt that we have enough data for real testing of statistical hypotheses in most cases, and such testing will make our choice less arbitrary. Indeed, there is nothing more statistically homogeneous than the residuals for the trend represented above by the polynomial of 14th order with each residual equal to zero. However, do you believe that it represents the real trend? In general, statistical testing of hypotheses is not a proof of their validity or invalidity; it only creates some basis for decision-making, which is still arbitrary. "A given degree of significance" means the probability to reject erroneously a tested hypothesis, usually called the null hypothesis. However, the null hypothesis "is never proved or established, but possibly disapproved" (Fisher 1935). In other words, if a hypothesis passes statistical testing at a given degree of significance, it means that we do not have enough evidence to reject it based on the criterion corresponding to the given degree of confidence. A number of different hypotheses able to pass the same test may exist. We know nothing about the probability of accepting the null hypothesis when it is false. However, this is essential for evaluating the uncertainty of our simulation results (see Sect. 3.4).

Dagan's suggestion to use "some prior information derived from similar sites" seems to be an attempt to include the only available element in a really existing ensemble and is a good idea. To do this, we must define what similarity between hydrogeological sites and impacts means, how it can be evaluated, and already know similar sites and their responses to the impact at hand. To my knowledge the method of geological analogy (Rozovsky and Zelenin 1975) is the only example of such an approach. Interesting conceptually, it has few practical applications, since it requires the existence of similar sites with similar impacts and already observed responses to those impacts.

Thus, we are able to make up a number of ensembles to which our site could belong. However, this does not change the situation: the choice of the ensemble remains an untested hypothesis.

3.2 Elements

Ensembles are collections of elements. The elements are bearers of properties or characteristics. Thus, when statisticians study the height, weight, or longevity of a population, the elements are human beings. When they study income, the elements can be families, and so on. To make the results more accurate and interpretable, statisticians make such ensembles as statistically homogeneous as possible: they partition the ensembles by gender, race, age, number of family members, level of income, etc. The fictitious analogous sites discussed in the previous section are also elements characterized by different random functions. Since geostatisticians consider all such elements to be analogous to the site at hand, let us restrict ourselves to properties within the site only.

In geology, and in particular in hydrogeology, the role of the element carrying a property is assigned to the representative elementary volume (REV). Following the established tradition (Kolomensky and Komarov 1964; Bear 1972; Brown et al. 2000), let us introduce the notion of REV using porosity. In principle, porosity can be measured on slices of media, applying the Bernoulli trail; that is, if a point selected at random falls into a pore, the result of the measurement x_i is assigned equal to 1 ($x_i = 1$); otherwise it is $x_i = 0$. If we repeat this procedure n times, than the porosity θ of the sample is evaluated as the mean of the measurements: $\theta = \sum_{i=1}^{n} x_i/n$. Its variance, $\sigma^2 = (\theta(1-\theta))/(n-1)$, decreases with increasing number of measurements. The standard procedure of evaluating the porosity on samples of finite volume is more convenient, since each such evaluation substitutes for manifold measurements on slices. Nevertheless, the variation of the porosity still depends on the sample volume. A possible pattern of the change of estimated mean porosity for samples of different volume is shown in Fig. 3.2. The sample volume for which the variance of the porosity becomes negligible is assigned as the REV. If we continue to increase the sample volume, the mean or mathematical expectation of the porosity can start changing again. These changes are usually attributed to the fact that the volume becomes too large and includes some heterogeneous

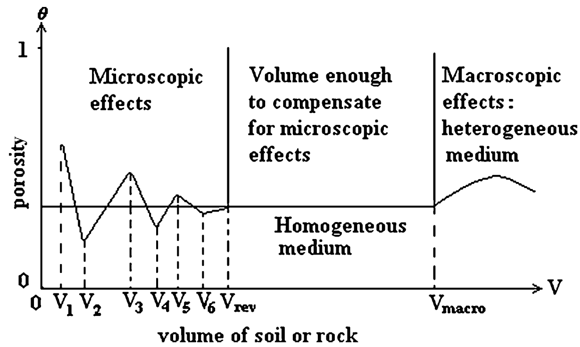

Fig. 3.2 Definition of representative elementary volume for porosity

macroscopically changes in the structure of the medium; it becomes statistically and geologically heterogeneous.

The notion of REV defines the element bearing a property, i.e., its point value, and makes the property continuous in space. It is possible that different representative elementary volumes exist for different properties. The minimum of those volumes can be considered as the REV for all pertinent properties.

In the case of porosity, changing the sample volume leads to change of the variance σ^2. This phenomenon is called by Rats (1968) a "scaling effect of the second kind." It is well known to statisticians (Yule and Kendall 1950). Some properties have "scaling effect of the first kind" (Rats 1968). The means of such properties depend on the volume of the samples on which they are measured. For example, the mean of the strength of soil and rock decreases with increasing sample volume (Kolomensky and Komarov 1964) and the mean hydraulic conductivity increases with increasing sample volume (Rats 1968). According to Bolotin (1965), the strength of a sample is defined by the weakest element of its structure. The probability of having such elements in a sample increases with sample size. Rats (1968) extended this explanation to hydraulic conductivity: the hydraulic conductivity is defined by the most conductive element in a sample. The probability of finding such structures within a sample is larger for larger samples. One of the Weibull probabilistic distributions relates the mean of the hydraulic conductivity obtained on samples of volume V with the mean conductivity of a reference sample of volume V_0. Thus, the results obtained by testing different volumes of soils and rocks may be different statistically even for statistically homogeneous media, just because of differences in the volume of samples, and this can cause some problems with defining the REV.

The notion of REV is convenient in laboratory studies when the volume of samples can be controlled. However, here we are most interested in cases in which we can control neither the volume nor the shape of the bearers of the obtained results, as happens, for example, in pumping tests. To deal with such situations, Rats (1968), Dagan (1986), and many other hydrogeologists have suggested a simple and straightforward approach. They introduce different scales of heterogeneity and use these scales as elements of corresponding ensembles. Thus, Dagan (1986), speaking about the hydraulic conductivity, says that a point on the *local scale* has dimension of order 10^{-1}–10^{0} m. These points are characterized by results obtained on extracted cores and by slug tests. At the *regional scale*, according to him, a point has dimension of the order 10^{1}–10^{2} m.

Such assignation of the elements carrying property values is arbitrary in essence. Thus, it is not clear why the results yielded on cores are of local and not laboratory scale. Pumping tests involve different volumes of soils and rocks, depending on geological settings, duration, patterns of the tests, and interpretation models. For example, 3-h, 3-day, 3-week, and 3-month pumping tests involve different volumes of geological media. Then the question arises: should we introduce different scales for the results of pumping tests of different durations, and if so, how many scales should we have and how should we define them? The results of pumping tests depend on interpretation models. We can arbitrarily change these and obtain different results and bearers of the hydraulic conductivity or transmissivity. For example, if we consider an aquifer as homogeneous and unconfined in the plane, and assign the boundary conditions at infinity, then the resulting hydraulic conductivity or transmissivity formally relates to the entire aquifer, which is not realistic. If we had a developed monitoring network, we could limit the infinity using the distances to the closest monitoring wells that do not respond to the pumping. Without such a network, we can do what geophysicists usually do, namely to call infinity the distance exceeding the thickness of the aquifer by ten times, or something similar. If we apply a different interpretation model, say a pumping test conducted near a river well connected to the aquifer, we may have a quite different situation. When the hydraulic conductivity and transmissivity are defined by model calibration, the elements bearing the results of calibration depend on the structures of the calibrated models and the formulation of the model identification problem (Gorokhovski 1977; Yeh and Yoon 1981; Yeh 1986).

The scales and their interaction are confusing, at least for me. So, it is interesting to see how geostatisticians deal with them. For example, Zimmermann et al. (1998) use in their work estimates of the hydraulic transmissivity at 41 boreholes obtained through slug tests, local pumping tests, and three regional-scale pumping tests lasting from 1 to 3 months. The obtained transmissivity values span seven orders of magnitude, from 10^{-7} to 10^{0} m^2/s. Nevertheless, all these transmissivity values are considered as a collection coming from the same ensemble (Zimmermann et al. 1998, Table 2a). Thus, the scaling is just ignored. I assume that this was done because it was impossible to infer serious statistical conclusions from the results obtained through three regional-scale pumping tests. The same happens if we separate slug tests and local pumping tests. (I do not believe that serious statistical conclusions can be supported by 41 available values either).

By the way, Zimmermann et al. (1998) state that "Large-scale pumping tests indeed suggest that narrow, relatively conductive fractured zones are possible in some areas." This is possible. On the other hand, the larger transmissivity values may be due to a scaling effect of the second kind. Another possible explanation is that the averaging of lower-scale hydraulic transmissivity values in the regional ones is not of statistical nature: the regional-scale transmissivity values are not weighted averages of the smaller-scale ones with nonnegative weights summing to one. Both of the above explanations contradict the statements of Dagan (1986), Moore and Doherty (2006), and many others that the results of regional pumping tests are averages of locally scaled properties. Review (1990) recognizes the existence of negative weights: “Negative weights (often, but not always) occur for points that are “shadowed” by closer points.” The authors do not explain what exactly “shadowed” means or why the negative weights occur. Isaaks and Srivastava (1989) relate the appearance of the negative weights in their Eq. 17.1 to the values of secondary data without any explanation of what the “secondary data” means. The appearance of the negative weighting factors follows also from Eq. 8.25 presented by Kitandis (1997), also without explanation. (The mechanism of the appearance of the negative weights is demonstrated in Chap. 5).

Unfortunately, the notion of an element in hydrogeological geostatistics is as vague as the notion of an ensemble. Both are “a matter of analytical convenience.”

3.3 Sampling at Random

Sampling at random is one of the most important requirements for making provable statistically inferences, but what is sampling at random? Gnedenko (1963) writes that “many authors have arrived at the conviction that in the case of infinite number of outcomes, no definition of probability can be given that is objective and independent of the method of calculation.” He gives several examples of problems which, depending on the operational definition of sampling at random, actually lead to different problems with different solutions, and describes the real-life situations relevant to each solution. One of them, called Bertrand’s paradox, is cited here.

The problem is formulated as following: A chord of a circle is chosen at random. What is the probability that its length exceeds the length of a side of the inscribed equilateral triangle?

Case 1 By consideration of symmetry, the direction of the chord can be fixed at point A in advance. The chords of this direction exceed the length of a side of the inscribed triangle if they intersect the diameter that is perpendicular to them within the interval CC'.The length of this interval is equal to the radius of the circle, r (Fig. 3.3, case 1). Since the diameter of the circle is $2r$, the probability for the chord length to exceed the side of the equilateral triangle is equal to 1/2.

Case 2 As in case 1, we can fix one end of a chord in advance. The tangent to the circle at this point and two sides of the inscribed equilateral triangle with vertex at this point form three angles, each equal to 60° (Fig. 3.3, case 2). Only the chords falling within the middle angle are favorable cases. Thus, by this method of computation, the probability we are looking for is equal to 1/3.

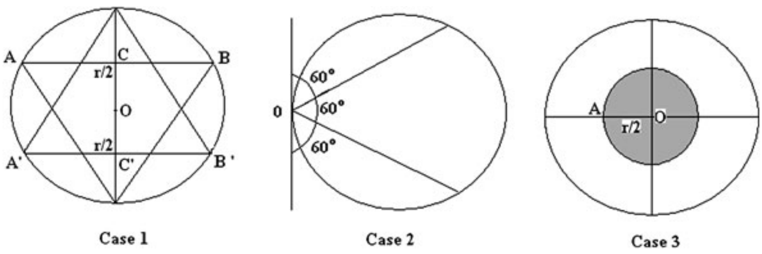

Fig. 3.3 Bertrand's paradox

Case 3 We also can fix the positions of a chord by indicating its midpoint position. For chords to exceed the length of a side of the inscribed equilateral triangle, the midpoint must lie within the concentric circle with radius $OA = r/2$ (Fig. 3.3, case 3). The area of this circle is equal to 1/4 of our circle. Therefore, the probability we are looking for is equal to 1/4.

Depending on how the notion "at random" is defined, we actually have three different problems with three different solutions. Gnedenko (1963) provides real-life situations relevant to each of these three formulations of the notion "at random."

Thus, good practice would dictate that, when formulating a geostatistical problem, the sampling at random must be defined operationally, and its relevance to the problem formulation must be demonstrated. This has never been done in hydrogeology. Moreover, the sampling systems in hydrogeology are almost never random; they are based on professional experience and understanding of hydrogeological surroundings. Thus, when prospecting for groundwater resources, hydrogeologists allocate wells where they anticipate to find water. They do not conduct pumping tests where low hydraulic conductivity is suspected. This is sound and effective hydrogeological practice. However, the results based on such sampling systems are not representative statistically: they are biased.

3.4 Probability Distributions

Almost all theoretical and practical developments of geostatistics in hydrogeology are based on the assertion that hydraulic conductivity and transmissivity have lognormal probabilistic distribution. This assertion is very convenient, greatly simplifying calculations. However, it reminds one of the well-known joke that physicists consider that the universality of the normal distribution of probability is a theorem proven by mathematicians, while mathematicians think that it is an empirical law established by physicists. Likely, hydrogeologists and geostatisticians consider the lognormality of hydraulic conductivity in the same way.

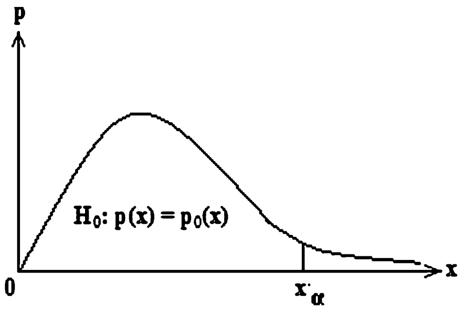

Fig. 3.4 Testing hypothesis H_0 based on a degree of confidence

In fact, according to Review (1990), there exist many different probability distributions of the hydraulic conductivity and transmissivity. Thorough studies conducted in the Soviet Union (Borevsky et al. 1973) have revealed that probability distributions of hydraulic conductivity can be divided into three, approximately equal groups: normal, lognormal, and those which could not be described as normal or lognormal.

As discussed above, the volumes characterized by values of hydraulic conductivity are known only if they are obtained in laboratory tests, whereas the elements characterized by hydraulic conductivity values obtained by slug and pumping tests are not. Their volume and shape depend on the duration of the tests and the geological surroundings. In which case, the hydraulic conductivity of what do the probability distributions describe?

The common assertion that the hydraulic transmissivity has the same distribution as the hydraulic conductivity just adds confusion. For example, in the case described by Zimmermann et al. (1998), both have lognormal distribution of probabilities. However, the transmissivity is a product of the conductivity and the thickness of the aquifer. Therefore, the thickness should have some special distribution for the product of the thickness and the conductivity to have the same kind of probability distribution as the conductivity. I have never heard about a study of the probabilistic distribution of the thickness of an aquifer or aquifers.

Statements about distributions of hydraulic conductivity are usually based on testing a hypothesis about its probabilistic distribution at "a given degree of significance." Let us consider this procedure more closely. Let us assume that we have an ensemble whose elements bear random values of property X which probability density function is $p_0(x)$ (Fig. 3.4). To test our hypothesis, let us call it H_0 and perform the following simple procedure. We assign some criterion x_α. Then, we sample the ensemble at random. The obtained sample is characterized by value x_s. If $x_s > x_\alpha$, we conclude that our hypothesis that X has the probability density function $p_0(x)$ is wrong and reject it. Otherwise, we accept the hypothesis.

In practice we usually assign not x_α, but α, the degree of significance,

$$\alpha = \int_{x_\alpha}^{\infty} p_0(x)\mathrm{d}x \tag{3.1}$$

and calculate x_α based on Eq. 3.1. In technical applications, the degree of significance is usually assigned as 0.1, 0.05, or 0.01. If our selection of the sample has been random, than the probability of obtaining $x_s \geq x_\alpha$ is small. We expect that an event with low probability is not likely to happen in a single experiment. However, it has happened. Therefore, our assertion that value x_s has low probability likely is wrong. So, we reject the hypothesis that X has the probability density function $p_0(x)$.

However, rare events happen from time to time, and rejecting hypothesis H_0 may be a mistake. The probability of such a mistake is α. The degree of significance is the probability of erroneously rejecting the hypothesis which we are testing when it is true. In doing so, we commit a so-called type I error. Obviously, assigning the degree of significance is arbitrary. If we are critical with respect to the hypothesis, we can increase α, moving our criterion x_α to the left. This makes rejecting the hypothesis more probable. If we like the hypothesis, we can decrease α and move x_α to the right. This decreases the probability of making a type I error. Anyway, by assigning some degree of significance we establish a criterion for recognizing whether the obtained evidence is sufficient to reject our hypothesis, and no more than this.

However, what does a degree of significance say about the possibility of committing a type II error, i.e., accepting hypothesis H_0 when it is wrong? The answer is: not much. Common sense suggests that, in our case, by moving x_α to the right and decreasing α we relax the condition to accept our hypothesis. Therefore, the probability, β, of committing a type II error is increased. If we increase α, moving x_α to the left, we increase the probability of a type I error and decrease the probability of a type II error. That is all. We cannot evaluate β in a quantitative way unless we have the probability density function $p_1(x)$ of an alternative hypothesis H_1.

Let us assume that we have an alternative hypothesis H_1 with probability distribution function $p(x) = p_1(x)$ (Fig. 3.5). Only one of these two hypotheses is true. The procedure for testing the hypothesis is the same as above. We assign a criterion. It seems to be natural, but not mandatory, to pick as the criterion value x_{01} for which $p_0(x_{01}) = p_1(x_{01})$. Then, we sample at random ensemble X and obtain the sample for which $x = x_s$. If $x_s > x_{01}$, we conclude that hypothesis H_0 is wrong, reject it, and consequently accept hypothesis H_1. If $x_s < x_{01}$, we accept hypothesis H_0, rejecting hypothesis H_1. The probability of erroneously rejecting hypothesis H_0, i.e., the probability of making a type I error, is

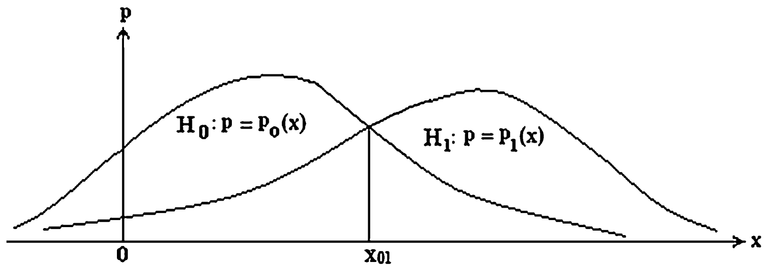

Fig. 3.5 Testing a hypothesis: simple alternative

$$\alpha = \int_{x_{01}}^{\infty} p_0(x)\mathrm{d}x. \tag{3.2}$$

The probability of erroneously rejecting hypothesis H_1 is

$$\beta = \int_{-\infty}^{x_{01}} p_1(x)\mathrm{d}x. \tag{3.3}$$

Erroneously rejecting hypothesis H_1, we erroneously accept hypothesis H_0. Therefore, β is the probability of making a type II error, to accept erroneously hypothesis H_0 when it is wrong. So the probability for hypothesis H_0 to be true is equal to $1 - \beta$. This value is called the power of the criterion.

Our choice of the value x_{01} does not consider the further use of the obtained result. Having some additional information, we can select a different value x_{01}. If we move x_{01} to the right, we decrease the probability of making a type I error, but increase the probability of a type II error. If we move it to the left, we get the opposite effect: we increase the probability of a type I error and decrease the probability of a type II error. If we knew the losses (loss_α and loss_β) associated with errors of both types, we could formulate the problem of finding x_{01} as a problem of optimization; that is, we could select x_{01} in such a way as to minimize the goal function representing the mathematical expectation of the losses:

$$\mathrm{loss} = \alpha\,\mathrm{loss}_\alpha + \beta\,\mathrm{loss}_\beta. \tag{3.4}$$

This provides about the most objectivity we can achieve, when performing hypothesis testing in the case of a simple alternative.

Hypothesis testing becomes more complicated in the case of many possible alternatives. It would be solvable still, if we could compile a complete list of alternatives weighted by their probabilities to be true. Say, we assume that the hydraulic conductivity has a lognormal distribution, but what is the complete list of mutually incompatible alternatives to our hypothesis? And how can we weight the hypotheses, including H_0, to be true?

The point here is that, when making a choice based on a given degree of significance, we cannot evaluate the uncertainty associated with the choice. We do not know the elements to which values of the hydraulic conductivity relate, and we cannot compile a complete list of the possible alternative probability density functions and objectively formulate the objective function for making this choice. Therefore, we never know the probability that the accepted hypothesis is false. Or coming back to the challenge of evaluating the uncertainty of the results of hydrogeological modeling, we never know the uncertainty associated with the acceptance of our hypotheses. This relates to all parameters involved in underground water flow.

3.5 Effective Hydrogeological Parameters

To produce predictions related to underground flow and contaminant transport based on solving the pertinent mathematical equations and their systems (mathematical models), we have to know the coefficients of the mathematical models continuously, that is, at each point of the geological object of interest and at each instant of the period of the predictions, as well as the corresponding initial and boundary conditions. Since this is impossible, simulation results never reproduce reality exactly. In the geostatistics approach the goal is to reproduce an average behavior of all processes of interest related to the underground flow: the hydraulic heads, fluxes, contaminant plume contours, travel time, etc. It is assumed that this can be achieved using some lump values of the pertinent parameters. Thus, instead of noncountable (infinitely large) sets of property values, small finite numbers of them can be used (Cooley 2004). These values are called effective parameters. Since the goal of the geostatistical approach is to predict some average behavior of the underground flow, it seems natural to use some statistics of the pertinent characteristics as effective parameters.

It was believed at an early stage of geostatistics development that the statistically inferred effective hydraulic conductivity is effective in a broad spectrum of hydrogeological situations, since "if there is no unique best effective hydraulic conductivity…, the predictive capability of the model must be questioned" (Gomez-Hernandez and Gorelick 1989). Dagan (1986), defining the effective conductivity as the value that satisfies exactly the Darcy law for uniform steady-state average flow, holds that the effective hydraulic conductivity, K_{ef}, is bounded by the harmonic mean,$K_H = \exp\left(\mu_Y - \sigma_Y^2/2\right)$, and the arithmetic mean,$K_A = \exp\left(\mu_Y + \sigma_Y^2/2\right)$, where μ_Y and σ_Y^2 are the geometric mean and the variation of the natural logarithms of the observed values of the hydraulic conductivity K:

$$K_H \leq K_{eff} \leq K_A. \tag{3.5}$$

He also holds that, for three-dimensional flow in isotropic media,

$$K_{\text{eff}} = K_{\text{G}}\left(1 + \sigma_{\text{Y}}^2/6\right), \tag{3.6}$$

where $K_{\text{G}} = \exp(\mu_{\text{Y}})$ is the geometric mean.

It is interestingly that, according to Dagan (1986), Eq. 3.6 "is of a rather academic interest," since "we generally measure directly a space average of K by pumping tests" and "under certain limiting conditions, yet to be elucidated in a quantitative manner, this space averaging is close to K_{ef}." The concept that the results obtained by pumping tests on some scaling level are averages of the hydraulic conductivity values belonging to the preceding scale level is shared by most geostatisticians (Review 1990; McLaughlin and Townley 1996; Cooley 2004; Moore and Doherty 2006, and many others). However, as mentioned above, the results of pumping tests depend on the chosen interpretation models, which are arbitrary in principle. It is hard to believe that the choice of the interpretation models does not affect the character of "the space averaging."

The concern of Gomez-Hernandez and Gorelick (1989) regarding the predictive capability of a model if there is no unique value of the effective hydraulic conductivity happened to be justified. Beven (1989) writes that many studies "have concluded that it is not possible to define a consistent effective parameter value to reproduce the response of a spatially variable pattern of parameter values." Neuman and Orr (1993) demonstrated that "an effective hydraulic conductivity does not generally exist." They also "demonstrated numerically that in two dimensional mean radial flow an effective hydraulic conductivity may increase from the harmonic mean of $K(x)$ near interior and boundary sources to the geometric mean far from such sources." However, contrary to the statement of Gomez-Hernandez and Gorelick (1989), the predictive capability of predictive models is not questioned by geostatisticians.

Cooley (2004), recognizing the absence of unique effective values of the hydraulic conductivity, explains it, as do many other geostatisticians, with the fact that hydrological mathematical models are nonlinear with respect to the hydraulic conductivity. To understand this, let us consider a simple example. Let some variable of interest q be a linear function of the property k:

$$q = ak + b.$$

Let k take values k_1 and k_2. Than, the arithmetic average value of q is

$$\bar{q} = \frac{ak_1 + ak_2 + 2b}{2} = \frac{ak_1 + ak_2}{2} + b = a\frac{k_1 + k_2}{2} + b = a\bar{k} + b.$$

So, we can evaluate the arithmetic mean value of $\bar{q}$ and its statistical characteristics by applying the arithmetic mean value $\bar{k}$ and its statistical characteristics.

Now, let variable h be a quadratic function of k:

$$h = ak^2 + b.$$

Then, the arithmetic mean value, $\bar{h}$, is not equal to its estimate $\hat{h}$ calculated with the use of the arithmetic mean $\bar{k}$:

$$\bar{h} = \frac{ak_1^2 + ak_2^2 + 2b}{2} = \frac{a}{2}\left(k_1^2 + k_2^2\right) + b \neq a\bar{k}^2 + b = a\left(\frac{k_1 + k_2}{2}\right)^2 + b = \hat{h}.$$

Indeed,

$$\bar{h} - \hat{h} = \frac{a}{2}\left(k_1^2 + k_2^2\right) - a\left(\frac{k_1 + k_2}{2}\right)^2 = \frac{a}{4}\left(k_1^2 - 2k_1k_2 + k_2^2\right) = \frac{a}{4}(k_1 - k_2)^2.$$

Unless $k_1 = k_2$ or $a = 0$, making h constant,$\bar{h} \neq \hat{h}$, due to the nonlinearity of the mathematical models. So, different variables of interest can require different effective values of the same parameters. Of course, this example is an oversimplification of real-life situations, just to demonstrate in the simplest way how nonlinearity works.

No doubt, the nonlinearity of hydrogeological problems contributes to the fact that the effective parameters are not universal. However, an even greater part in the nonuniversality of statistically effective parameters is played by the phenomenon of problem dependence of model identification, which in turn is related to the fact that the structures of geological models differ from the structures of real geological objects (see Chap. 4).

3.6 Meaning of Geostatistically Inferred Results

Let us assume that all our geostatistical assertions about the site of interest are true and that we have obtained true results. What do they mean really? For example, an insurance company evaluates the average longevity for a segment of population and does this correctly. However, can the company predict what will happen to a person with the average characteristics of a given segment of the population? The answer is no. The segment of population to which my parents and my talented colleague belonged had average longevity of about 60 years. My parents passed away at ages 89 and 92 years and my colleague at 40 years.

Meteorology, with its much longer historical records, numerous comparisons of statistical generalizations with real facts, and much better developed observational networks and predictive techniques than hydrogeology, makes a quite expressive illustration of this point. Thus, a 100-year flood event statistic refers to the disastrous floods which, in a long sequence of years, occur on average once per 100 years; that is, it has probability equal to 0.01 to happen during a 1-year period. Nevertheless, two such floods happened in California during just the first 3 months of 1995, and then again in 1997. The possibility that climate change or some other factors depriving the long previous series of observations of their statistical meaning for future predictions makes the situation even worse.

In the same way, the geostatistical approach, if all its assumptions are true, leads to results that represent the average response of a made-up imaginary ensemble. They do not relate to the unique object used to make up the ensemble, or to what may happen to that object.

3.7 Geostatistics and Uncertainty

As Hornung (1990) puts it, "One cannot substitute lack of theory and/or data by sophisticated mathematical models for parameter identification." Developing such complex theories as hydrogeological geostatistics, or proving new and beautiful theorems, is challenging and gratifying. However, how practical are those achievements? V.N. Tatubalin, a colleague of A.N. Kolmogorov and B.V. Gnedenko in the Department of the Probability Theory, Moscow State University, USSR, who often consulted hydrogeologists and geological engineers in the 1960s and 1970s, used to say: "You are looking for a razor. But considering amount and quality of your data, you would better learn to work with a chopper."

Shvidler (1963, 1964), one of the pioneers in the application of random functions to underground flows, gives the best (to my knowledge) practical example, applying them to oilfields consisting of 60–80 wells located on a relatively small territory. He describes the procedure of geostatistically solving the filtration problem in the following way (his notation is substituted with the one used in this text):

1. From experimental data, one realization of the random function $K(x)$ is constructed.
2. From one realization, the appropriate functional characteristics—mathematical expectation and autocorrelation functions of (the hydraulic conductivity) $K(x)$—are determined.
3. Based on them, sufficiently many realizations of $K(x)$ are constructed.
4. Any algorithm whatsoever for solving the corresponding boundary-value problem for each realization of $K(x)$ is applied.
5. From the set of boundary-value solutions obtained, the fundamental characteristics of the random function $h(x)$ are computed.

To realize steps 1–3, he applied the assumptions of stationarity of the observed random function $K(x)$, suggested later by Dagan (1986). To realize step 4, he applies different algorithms including analytical or numerical solutions, the method of small perturbations, the random walk, and the Monte Carlo simulations, all of them in deterministic mode. Step 4 provides also the solution of the problem of the nonlinearity of the original deterministic problem. In step 5, Shvidler usually restricted himself to calculating the mean and variation of the yield of the oil pumping wells. The latter was usually based on the Chebyshev inequality: if $\lambda > 1$ is an arbitrary positive real number, q is a random variable, $\bar{q}$ is its mean, and $\sigma_q$is its standard deviation, then the probability of the event $|q - \bar{q}| > \lambda\sigma_q$ is smaller than λ^{-2}, that is,

$$P\{\,|q-\bar{q}|>\lambda\sigma_q\}<\lambda^{-2}. \tag{3.7}$$

The Chebyshev inequality does not depend on the probabilistic distribution of the random variable q and permits evaluation of two-sided confidence intervals for a given confidence level and vise versa, though it overstates the confidence levels. For example, an arbitrary distributed variable q lies in the interval $\bar{q}\pm 3\sigma_q$ with probability close to 0.9.

Shvidler states also that it is necessary to have tens and in some cases even hundreds of observations for reliable derivation of correlation functions. (In his real-life examples, the number of wells is always above 60.) Since, in many cases, we do not have sufficient information for a valid determination of the statistical characteristics of the random functions, we have to choose between the deterministic and stochastic approaches. However, he writes: "It is quite obvious that the statistical model should be preferred as being more general." It may be, but not for me.

Shvidler (1963, 1964) never mentioned that the statistical approach provides provable estimates of the uncertainty of its results. He rather considers it as a way to systematize and optimize modeling: Steps 1–3 above are preparations for step 4, which is essentially deterministic. It is possible that the geostatistical approach can be useful in this sense sometimes, for example, in a context of model equifinality (Beven and Freer 2001). However, what is discussed here is not the comparison of the computational efficiency of the two approaches but the inability to obtain provable estimates of the uncertainty of the results of the engineering approach and, as if, the ability of the geostatistical one to provide such estimates.

It is a common and sound practice in mathematics to use convenient assumptions and methods such as Lagrange multipliers or perturbation methods to facilitate analytical solution of many problems. When analytical solutions are impossible, finite-difference and finite-element methods are convenient tools to yield numerical solutions. Statistical concepts and Monte Carlo simulations are sometimes used as a convenient tool to solve deterministic problems such as evaluating integrals and solving differential equations. The Buffon needle problem of the value of π estimation is a famous example of the application of the Monte Carlo method (Gnedenko 1963; Gentle 1985). However, all such applications include demonstrations that the employed conveniences actually lead to the solution of the original problem; that is, the yielded solutions converge to the true solutions if the number of experiments, or nodes in case of numerical methods, goes to infinity.

This is not the case for hydrogeological applications of geostatistics in which the word "random" is like the magic spell "open sesame": one proclaims whatever one wants as random and then is free to proceed. In geostatistics, analytical convenience means complete substitution of the problem needing solution by a vaguely related problem which seems easier to solve. The deterministic problem of finding space–time distributions of the hydraulic heads caused by a given impact within a given site is replaced by the problem of evaluating the average distributions of the hydraulic heads or fluxes belonging to a made-up ensemble. The reason for the substitution is the impossibility of estimating the error of the results from the deterministic formulation of the problem. To solve this new problem, an ensemble is made up which consists of undefined elements and actually even does not exist, random functions are applied to the phenomena which are not random, and many assumptions are employed which are not properly tested, or not tested at all, and "generally false and known to be false" (Morton 1993; Beven 2005).

The geostatistical approach may render the results acceptable practically. However, contrary to the statements of geostatisticians, it does not permit evaluation of the uncertainty of those results. Thus, one of their most power tools to overcome the nonlinearity of hydrogeological models and complications with defining the statistical distributions of the simulation results is Monte Carlo simulation. Let us forget that expressing the simulation result uncertainty in terms of levels of significance without evaluating type II error is meaningless. The main problem with such use of Monte Carlo simulations is that their object is a model itself but not its relation to the real world (Gentle 1985). Varying the parameters of a model, one can evaluate its sensitivity to those parameters, but no more than this.

I do not think that all this is news for geostatisticians, at least for those from the first generations. I cited above works of Dagan (1986) and Review (1990) where they stated directly that they introduce most of their assumptions not because they are true, but because they are convenient. However, Kitanidi (1997) motivates the next generation of geostatisticians, claiming that "because we cannot come up with a deterministic mechanism that explains variability, we postulate a probabilistic model," that common sense "is often the best guide," and that geostatistics is a "practical and reasonable way to use what we know in order to make predictions." He recognizes that the geostatistical technique may be misleading and should be avoided if certain assumptions are not met. Based on common sense, he suggests considering an assumption as met if it is reasonable, there is no evidence to the contrary, and the data do not discredit the assumption. All of these and even more have been already discussed above.

However, the two following suggestions are new. First, Kitandis (1997) suggests, based on common sense and the geostatistical tradition, to use Fourier decomposition "to grasp the concept of scale" for properties varying in space. The Fourier expansion representing a function as a sum of an infinite number of harmonics of different periods and amplitudes is a powerful and widely used tool in both pure and applied mathematics. However, if we take into consideration that about any trend, including linear and polynomial, can be subjected to Fourier decomposition and presented as a sum of an infinite number of harmonics of different periods and amplitudes, then it becomes obvious that Fourier decomposition has nothing to do with the concept of scale. Applying such logic, we can use the Taylor expansion to grasp the linear, quadratic, cubic, and further components (or scales?) of the regional trend. Mathematics permits describing trends as sums of the harmonics, but any periodicity has geological meaning if it is supported by geological evidence and considerations, not the other way round.

Second, Kitandis (1997) mentions a couple of times the principle of Occam's razor, that is, the use of the simplest empirical model consistent with the observed data. Taking into account how many assumptions the geostatistical approach involves, citing the principle of Occam's razor as one of the reasons for the geostatistical approach sounds at least ironic.

This chapter happened to be much longer than I expected, the reason being that, due to the brilliance of the leading geostatisticians, geostatistics has won the market, at least in terms of scientific publications. I speak without any irony about their brilliance. They have solved many difficult mathematical problems and obtained many beautiful results. Unfortunately, all this does not solve the problem of the uncertainty of the results of hydrogeological modeling, and the reason for this is the use of too many assumptions and postulates, most of which cannot be tested or are just not true. In the beginning of the application of geostatistics to hydrogeology, they honestly declared that those assumptions and postulates were introduced for convenience only. We do not hear much about the physical and geological meaning or the consequences of accepting such assumptions at present. Frequent use, and tradition, has made them as if valid. It seems that many geostatisticians have believed that geostatistics really overcomes the uncertainty of the groundwater modeling problem. They communicate their belief to the community of decision-makers, and there exists a great danger if the decision-makers believe them. On the other hand, if somebody has enough data and wants to use the geostatistical methods as a tool for interpolation and extrapolation of sparse data and does not pretend falsely that this methodology permits evaluation of the uncertainty in a provable way, the geostatistical approach is as good as the deterministic one. Although it is more cumbersome, the development of computational techniques and methods makes this factor less and less significant.

Statistical methods are a powerful instrument for organizing, sorting, and analyzing data, revealing whether the data support a hypothesis, or that their structure has peculiarities which may possibly change the comprehension of a site or a phenomenon. They are rather a starting point for developing conceptual geological models. They permit calculation of confidence intervals and many other statistics. However, all of them are conditioned by different assumptions, and the more assumptions that are introduced, the less must be the trust in the conclusions following from application of those assumptions.

In general, the situation with geostatistics is not so bad. Once a proponent of geostatistics asked me why I am against it, as "Nobody uses it in practice," he added. And this is true, as serious application of geostatistics to hydrogeological problems requires an amount of data that is not feasible to acquire physically and economically in most hydrogeological and environmental projects.

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Chapter 4
Model Identification

To predict responses of geological objects on man-made or natural impacts by applying mathematical methods, i.e., by solving differential or integral equations, the pertinent properties of the geological objects should be assigned continuously, that is, at each point of the objects and at each instant of the period of simulation, if the properties vary in time, besides maybe countable sets of points, i.e., isolated in space and time points. The boundary and initial conditions must be known in the same way. Unfortunately, only an infinitesimal part of the required geological information is available from direct observations and measurements. This information gap must be filled, and geological models have to do the job. They are a tool for interpolation and extrapolation of the sparse available data to all points of the geological objects of interest.

Geologists, with their understanding of geological surroundings, seem to be the best developers of geological models representing geological objects in simulations. However, as discussed earlier, those models are not exact copies of real geological objects. The results obtained by using geological models cannot reproduce simulation processes exactly. So, the goal of predictive simulation is to yield the best, in some predefined sense, possible results. To this end, the models must be furnished with the values of the model-governing parameters providing those results. Such parameters and their values are called *effective parameters*.

The engineering and geostatistical approaches differ in their way of assigning the effective parameters. Proponents of the engineering approach just know, from theirs and their colleagues' practical experience, which models and which values of their parameters, which may be some statistics, are best in a given situation. Geostatisticians apply more complicated statistical methods inherent to their general concept. Both approaches test and refine their choices of the effective model parameters, observing how they reproduce the available data.

This process of finding or refining predictive model parameters based on available observations on natural or induced hydrogeological phenomena is known as model identification, model calibration, historical matching, or site-specific

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_4,

validation. Model identification is often considered as inverse problem-solving (Yakowitz and Ducstein 1980; Yeh and Yoon 1981; Carrera and Neuman 1986; Yeh 1986; Hornung 1990; van Genuchten et al. 1990; Aster et al. 2005; Carrera et al. 2005; Moore and Doherty 2006; Dai et al. 2010). However, in general, the term "inverse problem" is not a synonym for the term "model identification" and its synonyms listed above (see Chap. 9).

At present, model identification is the most popular method for assigning the effective parameters of predictive hydrogeological models. The results of calibration are often considered as the strongest argument in support of a model's soundness. The faith in the model identification is based, at least in part, on the belief that the identified parameter values compensate automatically for unknown details. Flavelle (1992) writes: "The calibration (or tuning) of model can be described by a goodness-of-fit parameter which reflects how well the calibrated results match the observed data being simulated. This scalar parameter should incorporate the measurement uncertainty of the observations as well as the uncertainty in the model output." He also holds that "validation tests can also be designed simply to measure the accuracy of the predictions, without reference to a predetermined accuracy as a criterion for acceptance or rejection." The latter statement expresses, likely, Flavelle's belief that we can judge the accuracy of future simulations based on the accuracy of the calibration of predictive models.

Some other professionals, relaying on model identification as an effective tool, are more cautious. As cited in Chap. 2, De Marsily et al. (1992) emphasize that success in calibration "does not prove that the model will be correct for all circumstances, it only increases our confidence in its value." Indeed, there exist many facts that put in doubt statements such as those of Flavelle (1992). Thus, Yakowitz and Ducstein (1980) describe failures of several successfully calibrated models to predict the hydraulic head development on the same water intake. They explain the failures by incorrectness of the model identification, equating it to the inverse problem. Freyberg (1988), using numerical experiments, demonstrated that success in prediction may not be related to success in matching observed heads and that a good calibration alone may not lead to good prediction.

Based on general philosophical considerations and examples from hydrogeological modeling practice, Konikow and Bredehoeft (1992) claim that a site-specific validation "per se, is a futile objective," a point disputed by De Marsily et al. (1992). Beven (1989) goes even further, holding that use of calibration as a tool for setting model parameters is rather "an act of faith that is not based on sound physical reasoning." Oreskes et al. (1994) state: "Verification and validation of numerical models of natural systems is impossible," and so on.

Accepting the philosophical arguments of Beven (1989), Hornung (1990), Morton (1993), Oreskes et al. (1994), Oreskes (2004), and others that successful model calibration does not guarantee success of predictive simulations, it seems too much to claim that site-specific validation is "a futile objective." We should analyze every piece of available information. Model calibration is one of the tools for such analysis. Playing with different models and parameter values can help improve understanding of the geology and hydrogeology of the objects and their possible responses on natural or manmade impacts, and why a specifically site-validated model could become misleading in predictive simulations.

4.1 Incorrectness in Mathematics

The usual explanation for model identification yielding misleading results is that it is an ill-posed, incorrect, problem. This makes it worth discussing the mathematical notion of incorrectness in more detail.

A problem is *well-posed*, *correct*, if the three following conditions hold:

1. The problem has a solution.
2. The solution is unique.
3. The solution is stable (continuous), meaning that small errors in the data lead to small errors in the solution.

If at least one of the above conditions is violated, the problem is *ill-posed*, *incorrect*.

One of the main causes of incorrectness is observation and rounding errors, whose role can be seen from the following simple example:

Let us consider evaluation of a parameter A based on observation of the process described by the equation

$$x = A\mathrm{e}^{-2t}, \tag{4.1a}$$

where t and x are the independent and dependent variables. The solution of this inverse problem follows directly from Eq. 4.1a as

$$A = x\mathrm{e}^{2t}. \tag{4.1b}$$

The process described by Eq. 4.1a has asymptote $y = 0$ (Fig. 4.1), which makes processes with different values of the parameter A indistinguishable for large values of t. However, using good mathematical software, we can evaluate the parameter A for very large values of t. Thus, for $t = 250$,

$$x = 5\mathrm{e}^{-500} = 0.35622882033706 \times 10^{-216} \text{ and } x = 10\mathrm{e}^{-500} = 0.71245764067413 \times 10^{-216}.$$

Substituting these values for x into Eq. 4.1b yields correspondingly

$$A = 5.00000000000000 \text{ and } \mathrm{A} = 10.0000000000000,$$

solving our inverse problem more than satisfactorily.

However, as soon as errors of observation and rounding become commensurate with the observed values, we obtain the situation presented in Fig. 4.1. Assuming that the resolution of the figure corresponds to the accuracy of measurements y, we see that the measurements do not permit separation of $A = 5$ and $A = 10$ for large

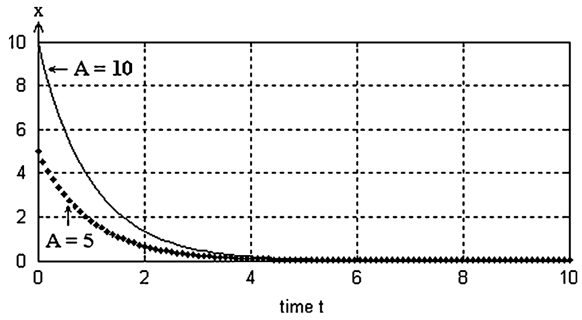

Fig. 4.1 Evaluating parameter A using observations on the process described by Eq. 4.1a

enough values of t. Conditionally, the problem is correct for $t < 3$ and incorrect for $t > 4$. There exists also a grey zone for $3 \le t \le 4$ where the correctness or incorrectness of the problem depends on the accuracy of the measurements.

This kind of situation is typical for hydrogeological processes developing from transient to steady-state filtration. Observation and calculation errors can make solving inverse problems impossible for some parameters, if observations are made close to the steady-state phase.

Let the actual behavior of the hydraulic heads be described by the function $h(x)$. However, what we observe is

$$h_{\mathrm{ob}}(x) = h(x) + \varepsilon(x), \tag{4.2}$$

where $\varepsilon(x)$ is the error of the observation at x. In many situations there is a need to evaluate the gradient of $h(x)$ based on observations $h_{\mathrm{ob}}(x)$. If $\varepsilon(x)$ is not differentiable (a random value, for example), $h_{\mathrm{ob}}(x)$ is not differentiable either. So, the problem of evaluating the gradient based on observations does not have a solution; it is incorrect.

Now, let us assume that the error is differentiable. For example,

$$\varepsilon(x) = A \sin(\omega x), \tag{4.3}$$

where A is the amplitude and ω is the frequency of the oscillations. Then, the gradient does exist and can be evaluated as

$$h'_{\mathrm{ob}}(x) = h'(x) + A\omega \cos(\omega x). \tag{4.4}$$

The upper boundary for the error in evaluating the gradient of h is $|A\omega|$. If the frequency ω is large, small errors in evaluating x can lead to large errors in evaluating $h'(x)$. This means that the problem of evaluating gradients based on observations can be ill-posed, even if the error is differentiable.

We can represent the observations differently, applying different differentiable approximations such as splines, polynomial regressions, etc. However, by applying different approximations based on the same observations, we may obtain different gradients. Moreover, we can find gradients when they do not actually exist.

One-dimensional steady-state filtration in a shallow homogeneous unconfined aquifer with constant hydraulic conductivity on a horizontal aquitard in the absence of recharge is described by the following differential equation, where $h(x)$ is the thickness of the aquifer, and K is its hydraulic conductivity, which is constant:

$$\frac{\mathrm{d}\left(Kh(x)\frac{\mathrm{dh(x)}}{\mathrm{dx}}\right)}{\mathrm{d}x} = 0. \tag{4.5}$$

If the boundary conditions in the model described by Eq. 4.5 are given as the aquifer thickness at the ends of the interval of interest [0, L], we cannot use the model to find the hydraulic conductivity of the aquifer: any value of the hydraulic conductivity satisfies Eq. 4.5, making the problem incorrect.

However, if one of the boundary conditions is given as the total flux Q, for example,

$$Q(0) = Q_0 = -Kh(0)\frac{\mathrm{dh(x)}}{\mathrm{d}x}\bigg|_{x=0}, \tag{4.6}$$

the model can be used to find the hydraulic conductivity K as

$$K = \frac{2Q_0 x}{h_0^2 - h^2(x)}. \tag{4.7}$$

Solution 4.7 is correct: it exists for all x that are not equal to zero, unique, and stable, since it is continuous with respect to h_0, $h(x)$, and Q_0. Actually we can use any two points, x_i and x_j within the interval [0, L] to find the hydraulic conductivity value as

$$K_{j,i} = \frac{2Q_0(x_i - x_j)}{h^2(x_j) - h^2(x_i)}. \tag{4.8}$$

However, let us assume that we have five observations over the thickness of the aquifer. This gives 10 possibilities to calculate the hydraulic conductivity, using Eq. 4.8. If our model, measurements, and calculations are absolutely accurate, then all values of $K_{i,j}$ are the same. However, if the model does not reproduce the real object exactly or the measurements and calculations carry errors, it is possible that we can have up to 10 considerably different values of the hydraulic conductivity. If the differences between those values exceed what could be expected based on the measurement errors, we have to recognize that our solution becomes not unique and the problem is ill-posed.

There are at least two obvious ways to reformulate the above problem to make it well-posed. One is to accept some statistics of the obtained values $K_{i,j}$ as the solution. On the other hand we can partition the aquifer according to the available observations and then consider that between the observations the aquifer is homogeneous. Thus, different hydraulic conductivity values characterize different parts of the aquifer, so we have a unique and stable solution of our problem but for a heterogeneous aquifer this time. In both cases we use ad hoc assumptions which usually cannot be verified.

Many inverse and model identification problems are reduced to solving systems of linear equations. Let us start with the following system:

$$\begin{aligned} x - y &= 1 \\ x + y &= 3 \end{aligned} \tag{4.9}$$

In the context of our discussion, the matrix of system 4.9 $A = \begin{Bmatrix} 1 & -1 \\ 1 & 1 \end{Bmatrix}$ can be interpreted as the characteristic of a model structure. Its right-hand vector $b = \begin{Bmatrix} 1 \\ 3 \end{Bmatrix}$ can be considered as observed data. The goal is to evaluate the parameters x and y, which are properties of the model. Note that these parameters, when interpreted geometrically, are the coordinates of the point of intersection of the lines represented by the equations of system 4.9.

The problem of evaluating parameters x and y is formulated correctly: it has a unique solution ($x = 2$ and $y = 1$) which is stable. Indeed, let us assume that the structure of the model and the observations carry errors such that, instead of system 4.9, we have system

$$\begin{aligned} 0.97x - 1.02y &= 0.99 \\ 1.04x + 0.95y &= 3.02 \end{aligned}$$

The unique solution to this system is $x = 2.03$ and $y = 0.96$. So, in response to reasonable inaccuracy of the model and the observations, we have reasonable errors in evaluating the parameters x and y.

Let us consider a different system

$$\begin{aligned} x - y &= 1 \\ 2x - 2y &= 3 \end{aligned} \tag{4.10}$$

System 4.10 does not have a solution at all: its determinant is equal to zero. Geometrically, the equations of system 4.10 represent two parallel lines which never intersect. Therefore, the problem of finding the parameters x and y for system 4.10 is ill-posed.

The system

$$\begin{aligned} 1.05x + 1.05y &= 1.05 \\ 0.98x + 0.98y &= 0.98 \end{aligned} \tag{4.11}$$

has infinitely many solutions, since both equations represent the same straight line and any values x and $y = 1 - x$ satisfy system 4.11. Therefore, the problem leading to system 4.11 is ill-posed.

The system

$$\begin{aligned} x + y &= 3 \\ 1.05x + y &= 4 \end{aligned} \tag{4.12}$$

is ill-posed also. The solution of this system is $x = 20$ and $y = -17$. However, if its coefficients carry measurement errors and system 4.12 takes, say, the form

$$\begin{aligned} 0.99x + 1.01y &= 3.01 \\ 1.06x + 0.98y &= 3.99 \end{aligned}$$

its solution becomes $x = 10.76$ and $y = -7.56$. Thus, small errors in measurements lead to considerable error in the solution. The reason is that the straight lines represented by the equations of system 4.12 are almost parallel and small errors in their coefficients lead to large errors in the coordinates of their intersection, given by the parameters x and y.

Since systems of linear equations play a considerable part in solving different problems, including hydrogeological ones, let us consider a general system of n linear equations

$$Ax = b, \tag{4.13}$$

where A is a square matrix of $n \times n$ size, x is a column vector of the unknowns, and b is a column vector of the observations (both of size $1 \times n$). To have a unique solution, matrix A must have an inverse matrix A^{-1}, such that $A^{-1}A = AA^{-1} = I$ (where I is the unit diagonal matrix whose nondiagonal elements are equal to 0 and whose diagonal elements are equal to 1). The matrix A^{-1} exists if the determinant of matrix A is not equal to zero, $|A| \neq 0$. Then

$$A^{-1}A\,x = x = A^{-1}b. \tag{4.14}$$

Discussion on the stability of the above solution requires the introduction of the notion of vector and matrix norms. Let us start with the definition of the vector norm.

A *vector norm* $\|a\|$ of vector a is a measure of the vector magnitude. It must be a real number having the following properties:

$$\begin{aligned} &\text{Iv} \quad \|a\| > 0 \quad \text{if} \quad a \neq 0 \\ &\text{IIv} \quad \|a\| = 0 \ \text{ if } \ a = 0 \\ &\text{IIIv} \ \|\mu a\| = |\mu| * \|a\| \quad \mu \text{ is a real number} \end{aligned}$$

If b is a vector with norm $\|b\|$ and its dimension is equal to the dimension of vector a, then the following properties hold:

$$\begin{aligned} &\text{IVv} \quad |ab| \leq \|a\| * \|b\| \qquad \text{Cauchy--Buniakowsky--Schwarz inequality} \\ &\text{Vv} \quad \|a + b\| \leq \|a\| + \|b\| \quad \text{Triangle inequality} \end{aligned}$$

There exist many different vector norms satisfying the above properties. The most popular matrix norms are the following:

$$\begin{aligned}
&\|a\|_1 = \sum_{i=1}^{n} |a_i| \qquad \text{norm 1} \\
&\|a\|_2 = \left(\sum_{i=1}^{n} a_i^2 \right)^{1/2} \qquad \text{norm or norm 2 or Euclidean norm} \\
&\|a\|_\infty = \max_{1 \le i \le n} |a_i| \qquad \text{norm infinity or maximum norm}
\end{aligned} \tag{4.15}$$

Since matrices are sets of vector columns or vector rows, it is natural to associate the matrix norms with the vector ones. Namely, for a matrix of size $n \times n$, some of the most often applied norms are defined as

$$\begin{aligned}
&\|A\|_1 = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{j,i}| \quad \text{norm 1 : the maximum magnitude of sum of matrix columns} \\
&\|A\|_F = \left(\sum_{j=1}^{n} \sum_{i=1}^{n} a_{j,i}^2 \right)^{1/2} \quad \text{Frobenius norm} \\
&\|A\|_\infty = \max_{1 \le j \le n} \sum_{i=1}^{n} |a_{j,i}| \quad \text{norm infinity : the maximum magnitude of sum} \\
&\qquad \text{of matrix rows}
\end{aligned} \tag{4.16}$$

As an example, let us consider the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

Corresponding norms are presented in Table 4.1.

The matrix norms share the properties of the vector norms, plus one more, related to the matrix–vector product (VIm):

$$\begin{aligned}
&\text{Im} \quad \|A\| > 0 \qquad \text{if} \quad A \ne 0 \\
&\text{IIm} \quad \|A\| = 0 \qquad \text{if} \quad A = 0 \\
&\text{IIIm} \quad \|\mu A\| = |\mu| * \|A\| \qquad \mu \text{ is a real number} \\
&\text{IVm} \quad \|AB\| \le \|A\| * \|B\| \qquad \text{Cauchy--Buniakowsky--Schwarz inequality} \\
&\text{Vm} \quad \|A + B\| \le \|A\| + \|B\| \quad \text{Triangle inequality} \\
&\text{VIm} \quad \|Ab\| \le \|A\| * \|b\|
\end{aligned}$$

It is assumed that matrices A and B and vector b in the above list of properties permit the operations involved. In particular, matrices are assumed to be square of size $n \times n$.

Table 4.1 Comparing different norms of matrix A

Norm 1	Frobenius norm	Norm infinity
18	16.8819	24

The notion of the coordinated vector and matrix norms permits evaluation of errors of the solutions of systems of linear equations (4.13). If matrix A and vector b carry errors, then system 4.13 becomes

$$(A + \Delta A)(x + \Delta x) = b + \Delta b, \tag{4.17}$$

where ΔA is the matrix of errors of the elements of matrix A, Δb is the vector of errors of the elements of vector b, and vector Δx is the errors of the elements of vector x. It follows from Eq. 4.17 that

$$\Delta x = A^{-1}(\Delta b - \Delta A x - \Delta A \Delta x). \tag{4.18}$$

Applying the norms and the triangle inequality to Eq. 4.18 yields

$$\|\Delta x\| \le \|A^{-1}\| \times \|\Delta b\| + \|A^{-1}\| \times \|\Delta A\| \times \|x\| + \|A^{-1}\| \times \|\Delta A\| \times \|\Delta x\|. \tag{4.19}$$

Inequality 4.19 can be reorganized as

$$\frac{\|\Delta x\|}{\|x\|} \le \frac{\lambda}{1 - \lambda \frac{\|\Delta A\|}{\|A\|}} \left(\frac{\|\Delta b\|}{\|b\|} + \frac{\|\Delta A\|}{\|A\|} \right), \tag{4.20}$$

where $\lambda(A) = \|A\| * \|A^{-1}\| \ge 1$ is the condition number. The condition number $\lambda(A) \ge 1$. Indeed,

$$\|A^{-1}A\| = \|I\| = 1 \le \|A^{-1}\| * \|A\| = \lambda. \tag{4.21}$$

Inequality (4.20) relates the relative errors of the solution to system 4.13 and the relative errors of the initial data of matrix A and vector b. The system is well-conditioned if$\lambda \approx 1$ to 10. A system is ill-conditioned if $\lambda \gg 10^2$–10^3. There exists the gray zone $10 < \lambda < 10^3$ within which the solution to linear systems may remain stable. Inequality 4.20 is meaningful if$\lambda \frac{\|\Delta A\|}{\|A\|} \le 1$. This implies that the ratio $\frac{\|\Delta A\|}{\|A\|}$ must be considerably smaller than 1. This requirement is practical enough, since there is no sense to working with an inaccurate system 4.13.

Note that the formulation of incorrectness includes the absence of *a mathematical solution*. It sometimes happens that a mathematically correct solution is physically incorrect, for example, a negative hydraulic conductivity. Such a situation is easily recognizable and could be rejected or accepted depending on how the physically incorrect solution is intended to be used (see Chaps. 6–9 for more details). It may also happen, as shown in the following chapters, that a solution looks physically correct but is incorrect geologically, being out of the actual property value range. Such a kind of incorrectness, let us call it *geological incorrectness*, is difficult if possible to recognize, though it could lead to catastrophic consequences.

4.2 Regularization of Ill-Posed Problems

The notion of correctness with respect to inverse problem formulations came from the application of mathematics to the study of properties of natural objects and impacts to which the objects are or were subjected. Real physical objects have unique real property distributions and, if the properties change in time, at each given instant. Each object has a unique response to a given impact. The response should depend continuously on small changes of the property values and impacts. Therefore, the inverse problem, using the observed data, must provide those unique distributions of the actual property distributions, and the impacts and initial and boundary conditions when they are needed. (There may be natural processes that are inherently instable. They are not discussed here).

At the time of the discovery of the existence of mathematically incorrect problems, it was natural to think that the incorrectness was caused by unfortunate formulations of pertinent problems. However, it later became obvious that there are many meaningful problems that are inherently incorrect. Most problems of geophysical and hydrogeological data interpretation are of this kind. (It is interesting to note that there are no processes in nature corresponding to inverse problems or model identification in geophysics and hydrogeology). As soon as this became clear, many methods to treat incorrect problems were developed. Those methods reformulate incorrect problems as correct ones. Discretization of the hydraulic conductivity in the previous subsection can be considered as such a method. Numerical differentiation of function 4.2 can be interpreted as such a method also. Indeed, if the locations of the observations $h_{\text{ob}}(x_i)$ are such that $x_{i+1} - x_i = x_i - x_{i-1} = \Delta x$, the derivative of $h_{\text{ob}}(x_i)$ can be evaluated as

$$h'_{\text{ob}}(x_i) \approx \frac{h_{\text{ob}}(x_{i+1}) - h_{\text{ob}}(x_{i-1})}{2\Delta x}.$$

As mentioned above, we can also apply splines, different regressions, and many other methods to obtain the derivative $h'_{\text{ob}}(x_i)$. However, attention is required here, as different methods can provide different values of the derivative $h'_{\text{ob}}(x_i)$. Also, as mentioned above, we can find the derivative even where it does not exist.

One of the most popular and thoroughly developed methods for converting incorrect problems into correct ones is Tikhonov regularization (Tikhonov and Arsenin 1977; Allison 1979; Aster et al. 2005). Applied to inverse problems, it consists of looking for the set of parameters that minimizes the functional

$$\beta = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(h_{\text{ob}}\left(x_i, t_j\right) - h\left(x_i, t_j, P\right)\right)^2 + \lambda \sum_{k=1}^{K} \left(P_k - P_{0,k}\right)^2. \tag{4.22a}$$

In Eq. 4.22a, $h_{\text{ob}}(x_i, t_j)$ is the observed value at the point with coordinate x_i at instant t_j. The simulation results are represented by $h(x, t, P)$, where $P = [P_1, P_2, \ldots, P_k, \ldots, P_K]$ is the list (vector) of parameters governing the simulation process, $P_0 = [P_{01}, P_{02}, \ldots, P_{0k}, \ldots, P_{0K}]$ is an a priori guess for the unknown values of parameters P, and λ is a small positive number called the regularization parameter. It is often assumed that $P_0 = 0$, meaning that all parameters in the a priori guess are equal to zero. Then, functional 4.22a can be rewritten in the form

$$\beta = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(h_{\text{ob}}\left(x_i, t_j\right) - h\left(x_i, t_j, P\right)\right)^2 + \lambda \sum_{k=1}^{K} P_k^2. \tag{4.22b}$$

Tikhonov regularization is a combination of least-squares regression with penalties for poor a priori guessing. Different forms of the penalizing term are also possible. In particular, it can be constructed to penalize larger values of derivatives of the model $h(x, t, P)$ to provide smoother solutions, so the penalizing term is often called the smoothing term. There exist statistical interpretations of Tikhonov regularization. They require additional assumptions on the statistical characteristics of the observations and the model itself, and are not discussed here.

Regularization substitutes one problem with another. Different regularizations of the same problem result in different problems having different solutions. Sophisticated regularization methods, such as Tikhonov regularization, converge to true solutions if the model subjected to regularization is true and adequate, and the noise, the random errors in observations and calculations, is the only complicating factor. However, all geological models are knowingly false (Morton 1993; Beven 2005). For example, the numbers of model parameters and the parameters governing the actual processes are different usually. What regularization means and achieves, if applied to false models, is disputable. It may be a proper moment to cite V. N. Tatubalin again (Sect. 3.7): "You look for a scalpel, but with such data as you have, you should rather learn to work with a chopper." He meant geostatistics, but it seems to be true with respect to regularization as well.

4.3 Problem Dependence of Model Identification

The problem dependence of model identification means that the results of identification depend on the formulation of the model identification problem. This phenomenon is commonly recognized and often cited (Gorokhovski 1977; Yeh and Yoon 1981; Carrera and Neuman 1986; Kool et al. 1987; Hornung 1990; van Genuchten et al. 1990). Practicing hydrogeologists always knew, for example, that the results of pumping test data interpretation depend on the interpretation models, and that it is possible to infer different, sometimes considerably different, hydraulic conductivities and transmissivities based on the same data. What is surprising is that problem dependence is actually ignored in practical applications and theoretical developments of model identification. Commonly it is referred to as some kind of nuisance along with the recommendation to maintain caution. Thus, Yeh and Yoon (1981) write: “In order to obtain physically meaningful parameter estimates, caution must be exercised.” Hornung (1990) requires lengthy discussion on the coupled predictive and inverse problem and “a thorough knowledge of the difficulties involved,” as if such discussion and knowledge are enough to overcome the problem dependence. Batu (2006), citing Mercer and Faust (1981), writes “Confidence in predictive results must be based on (1) a clear understanding of model limitations; (2) the accuracy of the match with the observed historical behavior; and (3) data reliability knowledge about aquifer characteristics.”

Hornung (1990), by the way, makes an excellent point, coupling predictive and model identification problems explicitly. Indeed, the goal of model identification is to find the parameters of a geological model, the effective parameters, which reproduce observations best in some predefined sense. When the set of parameter values is found, it furnishes the same structural geological model to solve the coupled predictive problem. However, predictive problems differ from the corresponding problems of identification nearly always. The differences can include the size and shape of the objects, impacts, boundary conditions, and monitoring networks. Often models calibrated under steady-state conditions are applied to predicting transient flows. It sometimes happens that the goals of calibration and prediction are different: a model that is calibrated based on observations on hydraulic heads is applied to find streamlines that are not observable directly. If a model were an exact copy of the pertinent geological object, than the model identification made once would be effective with respect to any predictive problem related to the object. However, models are not exact copies of geological objects, and this causes the problem dependence. Namely, the effective set of model parameters providing the best prediction of one kind, say, water table elevations, may not be and often is not the best one for a different kind of prediction, say, of streamlines (Beven 1989; Neuman and Orr 1993; Cooley 2004). Moreover, values of the effective parameters can change with time, without any changing in the simulation problem formulation (see Chap. 7).

Let us consider a simple and transparent example: a confined aquifer consisting of two homogeneous bodies, one with hydraulic transmissivity T_1 and the other T_2 (Fig. 4.2). In the initial state the aquifer has uniform distributions of the hydraulic heads $h(x, 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L$ jumps instantly to $h(2L, 0) = H_{2L}$ and then remains unchangeable: $h(2L, t) = H_{2L}$. At $x = 0$ the hydraulic head does not change: $h(0, t) = H_0$. The jump of the hydraulic head at $x = 2L$ initiates change of the aquifer hydraulic heads. We wish to predict this process based on a homogeneous model of the aquifer with the constant effective hydraulic transmissivity $\hat{T}$, whose value is to be found.

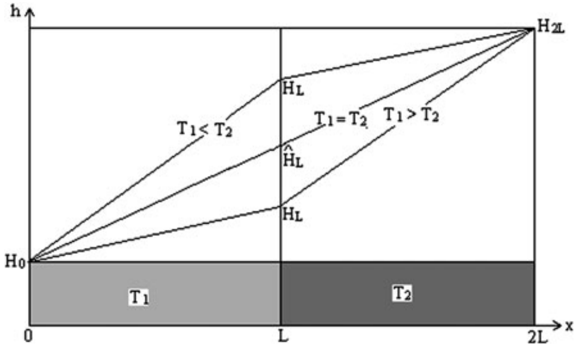

Fig. 4.2 Modeling a confined aquifer with a homogeneous model

The simulated process of developing the hydraulic heads in this case when neither sources nor sinks are present in interval [0, 2L] is described by equation

$$S\frac{\partial \hat{h}(x,\, t)}{\partial t} = T\frac{\partial^2 \hat{h}(x,\, t)}{\partial x^2} \tag{4.23}$$

where $\hat{h}(x,\, t)$ are the simulated hydraulic head at point x and instant t, T is the hydraulic transmissivity of the homogeneous model and S is its storativity which is assumed known and equal to 0.1. Assume also that observing the process during some not long period of time, we found the effective value of the model transmissivity $\hat{T}$.

To see what will happen to our prediction with the use of the found effective transmissivity $\hat{T}$, let us consider the steady-state distributions of the simulated $\hat{h}(x,\, t)$ and actual $h(x,\, t)$ hydraulic heads $h(x,\, t)$ when the process will reach the steady state. Then the left-hand part of Eq. 4.23 becomes zero, and the effective transmissivity, being concealed, disappears from the equation. Thus, the steady-state distribution of the simulated hydraulic heads is described by equation

$$\frac{d^2\hat{h}}{dx^2} = 0$$

which does not depend on the transmissivity. With the boundary conditions assigned as

$$h(0) = H_0 \text{ and } h(2L) = H_{2L}, \tag{4.24}$$

the solution to the simulated hydraulic heads $\hat{h}(x,\, t)$ is

$$\hat{h}(x) = \frac{H_{2L} - H_0}{2L}x + H_0. \tag{4.25}$$

Solution 4.25 corresponds to the straight line (H_0, H_{2L}) in Fig. 4.2 with

$$\hat{H}_L = \frac{H_{2L} + H_0}{2}. \tag{4.26}$$

Actually the steady-state filtration in the heterogeneous aquifer consisting of two geological bodies with the hydraulic transmissivities T_1 and T_2 is described by two functions: left ${}_{lft}h(x)$ within interval [0, L] and right ${}_{rgt}h(x)$ within interval [L, 2L]. The functions are solutions of the differential equations

$$\frac{d^2\left({}_{lft}h(x)\right)}{dx^2} = 0 \text{ and } \frac{d^2\left({}_{rgt}h(x)\right)}{dx^2} = 0 \tag{4.27}$$

under the outer boundary conditions: ${}_{lft}h(x) = H_0$ and ${}_{rgt}h(2L) = H_{2L}$. There exist also the inner boundary conditions on continuity of the hydraulic heads and the flux at $x = L$:

$${}_{lft}h(L) = {}_{rgt}h(L) \quad \text{and} \quad T_1 \frac{d_{lft}(h(x))}{dx}\bigg|_{x \to L} = T_2 \frac{d_{rgt}(h(x))}{dx}\bigg|_{L \leftarrow x}. \tag{4.28}$$

The conditions connect the solutions of Eq. 4.27 which are

$${}_{lft}h(x) = \frac{H_L - H_0}{L} x + H_0, \quad 0 \le x \le L \tag{4.29a}$$

$${}_{rgt}h(x) = \frac{H_{2L} - H_L}{L}(x - L) + H_L, \quad L \le x \le 2L \tag{4.29b}$$

where the unknown HL is the same for both solutions (the first condition 4.28). To find HL, the condition on continuity of the flux (the second Eq. 4.28 should be applied. Since functions ${}_{lft}h(x)$ and ${}_{rgt}h(x)$ are straight lines, their derivatives are equal to their slopes.

So, we can rewrite the second Eq. 4.28 as

$$T_1 \frac{H_L - H_0}{L} = T_2 \frac{H_{2L} - H_L}{L}. \tag{4.30}$$

Solving Eq. 4.30, we obtain

$$H_L = \frac{T_1}{T_1 + T_2} H_0 + \frac{T_2}{T_1 + T_2} H_{2L}. \tag{4.31}$$

So the steady-state hydraulic head H_L at the midpoint $x = L$ is the average of H_0 and H_{2L} weighted according to the actual hydraulic transmissivities. The equality $\hat{H}_L = H_L$ is true only if the aquifer is homogeneous ($T_1 = T_2$). If $T_1 < T_2$, then $H_L < \hat{H}_L$. If $T_1 > T_2$, then $H_L > \hat{H}_L$ (Fig. 4.2). The magnitude and sign of the deviation of $\hat{H}_L$ from the observed value H_L depend on H_{2L} and H_0, the ratio T_2/T_1, and time.

Calibrating the homogeneous model in the transient regime can permit the simulation results to fit the observation satisfactorily for some period of time. Then, the simulated and actual hydraulic heads will start diverging inevitably. If the calibration period is short, we may not see the divergence, but it makes itself known later.

The point of this simple example is obvious. The effective parameters of the simplified models may not and usually do not compensate for the unknown. We cannot evaluate the error of the simulation results yielded by our homogeneous model even in our simple case. It is possible that something like this caused the failures described by Yakowitz and Ducstein (1980). Unlucky simulation models could be the source of failures described by Kola (1984), Lerner (1985), Kerr (1993), and many others. However, in the presented case, the homogeneous model can be applied successfully for solving our predictive problem. To this end, the effective hydraulic transmissivity must vary in time (see Chap. 7).

4.4 More Complex Model Versus Less Complex One

That all models are false is no news. Practicing hydrogeologists know also that those false models often provide practically acceptable results. Otherwise modeling would not have any sense at all. Nevertheless it seems interesting to illustrate this contradiction (false models and acceptable results) on a simple real-life example. However, our notions on real geological objects are not more than models, and as such they are false. The only option left is to compare the results yielded by a more complex model, considering it as if true, and a less complex which is undoubtedly false. It is desirable to find a simple and well-studied object to make the comparison simpler.

The Borden landfill (Ontario, Canada) seems appropriate for such an exercise. It was in operation from 1940 to 1976. The contaminant plume in the shallow aquifer below the landfill was the subject of detailed investigations that lasted from 1974 to 1980. The simplicity of the site as a hydrogeological object, the sharply delineated plume, and the relatively large amount of data make the Borden site a suitable object for testing different approaches and models, as has been done more than once (Frind et al. 1985; Frind and Hokkanen 1987; Batu 2006).

The more complex model is the model applied by Frind and Hokkanen (1987). They simulated two-dimensional steady-state flow in the Borden aquifer in terms of streamlines. Correspondingly, the boundary conditions are assigned as specific fluxes normal to the object's boundaries. The main goal of their model calibration is to find the specific fluxes on the boundaries of the Borden site that provide the best reproduction of the observed streamline. (As discussed below, only one streamline can be considered as observable within the Borden site. Likely, the hydrogeological part of the model had been calibrated by reproducing that streamline.) Then, the obtained results, the recharge pattern and the streamlines, were applied to solve the mass transport problem.

The competing model is the D1_Flow model developed by the US EPA (Gorokhovski and Weaver 2007). It is a screening-level model numerically simulating one-dimensional steady-state flow in shallow unconfined aquifers on an arbitrarily shaped base. The model permits evaluation of water table, streamlines, and time for contaminants to travel to selected locations. Being simple in terms of data preparation and operation, it saves considerable resources and cost. The D1_Flow model is based on the Dupuit-Forchheimer assumption that the Darcy

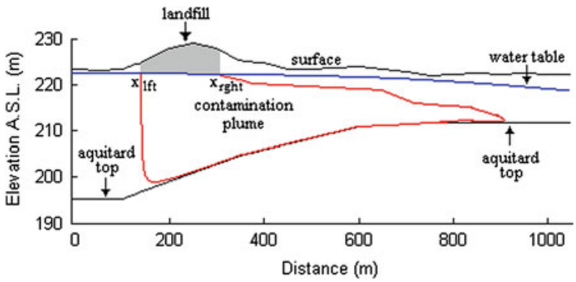

Fig. 4.3 Cross-section of the Borden landfill site

velocity is horizontal (i.e., that its vertical component can be neglected). This assumption simplifies the mathematical description of the underground flow considerably. The D1_Flow model has been validated thoroughly on available, not numerous, analytical solutions for a shallow aquifer on horizontal and sloppy (Polubarinova-Kochina 1962) bases. The results are more than satisfactory. The Borden site object has been chosen for validating the D1_Flow model on a real-life object (Gorokhovski and Weaver 2007).

Compared with the more physically sound, two-dimensional model by Frind and Hokkanen (1987), the D1_flow model is undoubtedly false: it simulates the flow as one-dimensional when it is actually at least two-dimensional, and uses the knowingly false Dupuit-Forchheimer assumption and the physically controversial method of calculating two-dimensional streamlines by a one-dimensional model, as suggested by Strack (1989) and described in Sect. 4.4.3. The model of Frind and Hokkanen (1987) does not need these assumptions.

The main goal of the D1_Flow model calibration below is to demonstrate that simple and by definition false models can yield results comparable to the results of more complicated and physically sound models such as that of Frind and Hokkanen (1987). Unfortunately, the factual data used by Frind and Hokkanen (1987) in calibrating their model as well as the accuracy of reproduction by their model of the corresponding observations were not available. For this reason, only the results obtained graphically from their publication are used in the D1_Flow model calibration. A byproduct of the D1_Flow model calibration below is explicit demonstration of the problem dependence of model identification. Frind and Hokkanen (1987) deal with this phenomenon, though without mentioning it.

4.4.1 Short Description of the Borden Landfill

The unconfined aquifer under the Borden landfill consists of beds and lenses of fine-, medium-, and coarse-grained sand overlying an extensive deposit of clay and sandy silt. The 10 ppm outline of chloride is chosen as the boundary of the contamination plume. The longitudinal cross-section of the site with the water table, the contaminant plume, and the aquitard surface (Fig. 4.3) was obtained

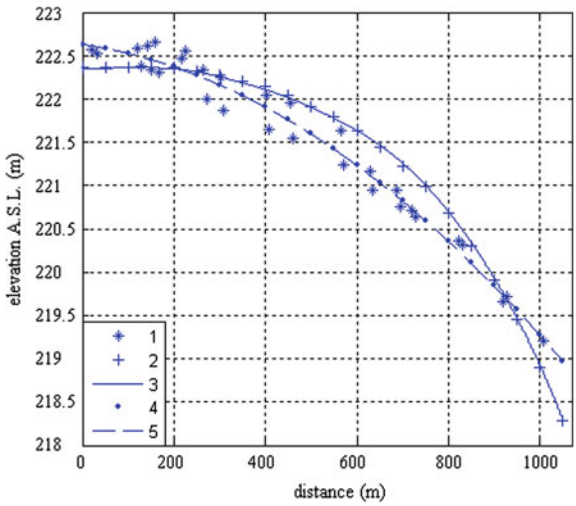

Fig. 4.4 Observed, assigned, and calibrated water tables: *1*-observations, *2*-water table assigned by Frind and Hokkanen (1987), *3*-reproduction of the water table of Frind and Hokkanen (1987), by D1_Flow model, *4*-water table approximated by regression 4.32, *5*-water table reproducing regression 4.32 by the D1_Flow model

graphically from Frind and Hokkanen (1987). The hydraulic conductivity of the Borden aquifer was assigned based on pumping and permeability tests as equal to 10.11 m/day in the horizontal direction and 5.05 m/day in the vertical direction. (Being one-dimensional, D1_Flow uses only the horizontal hydraulic conductivity in simulation of the Borden aquifer).

4.4.2 Simulating the Water Table

Frind and Hokkanen (1987), simulating the contaminant plume development within the Borden site, assume that the flux in the Borden aquifer is steady state. Their problem formulation requires that the boundary conditions be stable as well as the boundaries themselves. In particular, they assumed that the water table and precipitations do not change in time. In reality, the water table is affected by seasonal changes of precipitation. Thus, the first task to be addressed is to assign as if the long-term average steady-state water table. Frind and Hokkanen (1987) write "The aspect of the water table has been addressed by Frind et al. (1985)," who in turn resolve the issue by stating: "The water table boundary was obtained visually drawing a smooth curve through the relevant water level points." [By the way, Fig. 15 of Frind et al. (1985) and Fig. 4 of Frind and Hokkanen (1987) reveal that the water tables used in those works differ by up to 0.6 m] .The "relevant points" are the factual observations in April and December 1979. The water table thus assigned is arbitrary in essence. Besides, it is biased with respect to the available observations (Fig. 4.4). However, it is likely that the water table was an intermediate and not decisive part of their calibration processes. Their final goal was "matching streamlines to the observed plume" (Frind et al. 1985).

Table 4.2 Recharge patterns according to Frind and Hokkanen (1987), and the D1_Flow model (cm/year)

Interval (m)	0–140	140–300	300–600	600–800	800–1,050
Frind and Hokkanen (1987)	15	55	15	45	10
D1_Flow model	15	55	10	50	12

Table 4.3 Recharge pattern calculated by Eq. 4.33 and assigned by Frind and Hokkanen (1987) (cm/year)

Interval (m)	0–140	140–300	300–600	600–800	800–1,050
Equation 4.33	34	9	−1.6	2.7	−10

The D1_Flow model was calibrated with respect to the water table of Frind and Hokkanen (1987). The goal was to reproduce their water table by varying piecewise-constant recharge rates within the recharge pattern structure presented by Frind and Hokkanen (1987). The boundary conditions are assigned in the water divide at $x = 135$ m, where the water table elevation is 222.36 m and the total flux Q is zero. The choice of the boundary conditions is based on the figures of Frind and Hokkanen (1987), and supported by their boundary conditions. Indeed, the specific flux on the boundary at $x = 0$, where the thickness of the aquifer is about 30 m, is assigned as −70 cm/year. The recharge rate in the interval [0, 140] m is assigned as equal to 15 cm/year. The water table divide seems to be somewhere close to but not exceeding 140 m, since there is no evidence of a contaminant up-gradient to the landfill. The recharge pattern provided by the simple D1_Flow model (Table 4.2) reproduces the water table of Frind and Hokkanen (1987), with error magnitude less than 5 cm (Fig. 4.4), i.e., satisfactorily accurately.

It is interesting to note that, if 1979 were not a special year with respect to the long-term precipitation regime for the Borden site, it could be reasonable to present the long-term steady-state water table as some averaging of the observations in April and December. The least-squares method applied to those observations yields the following regression equation for depicting the water table:

$$r\hat{H}(x) = -2.5725 \times 10^{-6}x^2 - 7.7991 \times 10^{-4}x + 222.5731\,\mathrm{m} \tag{4.32}$$

(Other regression presentations of the water table are possible also) .The water table described by Eq. 4.32 is presented in Fig. 4.4. The corresponding total flux is described by equation

$$\begin{aligned} r\hat{Q}(x) &= K\frac{\mathrm{d}(rH)}{\mathrm{d}x}(rH(x) - Y(x)) \\ &= K\left(5.145 \times 10^{-6}x + 7.7991 \times 10^{-4}\right)(rH(x) - Y(x))\,\mathrm{m}^2/\mathrm{day}, \end{aligned} \tag{4.33}$$

where K (m/day) is the hydraulic conductivity. The water table simulated by the D1_Flow model and based on the piecewise recharge rate calculated by Eq. 4.33

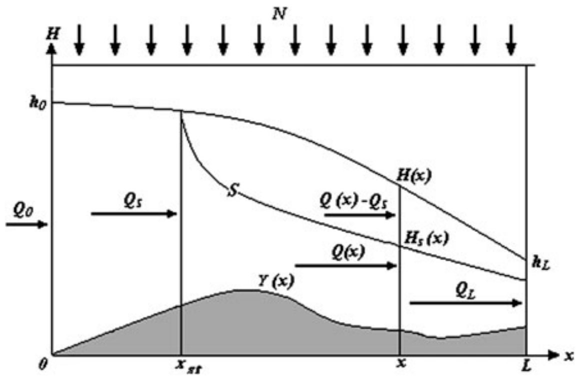

Fig. 4.5 Streamline calculation: $H(x)$, $H_S(x)$, $Y(x)$, and $Q(x)$ are the elevations of the water table, streamline and aquifer base, and the total flux at location x, $N(x)$ is the recharge, S is the streamline $[Q_S = Q(x_{st})]$

(Table 4.3) reproduces the water table depicted by Eq. 4.32 with error magnitude less than 4 cm. Interestingly, Frind et al. (1985) obtained a negative recharge rate, −30 cm/year, for x greater then 700 m, although the "slightly modified" recharge pattern of Frind and Hokkanen (1987) does not contain negative recharge rates (Table 4.2).

Note that the assumption about the existence of the water divide in the long-term average steady-state flow system makes the flow in the Borden aquifer three dimensional. It could be considered two dimensional along the axis of symmetry, if such an axis exists. Likely, Frind et al. (1985), and Frind and Hokkanen (1987), assume this implicitly.

The two observations above are just digressions. Since the goal is to demonstrate that the simple, and false, model D1_Flow is able to reproduce the results obtained by the complex model of Frind and Hokkanen (1987), we continue working with the data used and obtained in the process of calibration by Frind and Hokkanen (1987).

4.4.3 Calibration with Respect to the Streamlines and the Arrival Time

As mentioned above, Frind and Hokkanen (1987), following Frind et al. (1985), assigned their water tables arbitrarily and then calibrated the flow system based on the plume configuration "matching streamlines to the observed plume" (Frind et al. 1985). There are only two streamlines which could be considered as if observed: the upper and bottom boundaries of the plume. The bottom boundary is not informative, since the corresponding streamline starts near the water divide and seepage along this streamline is extremely low, theoretically equal to zero. Thus, only the sharply outlined upper boundary of the Borden plume can be interpreted as the streamline to be used in calibration.

Calibrating their model with respect to the streamlines, Frind and Hokkanen (1987), following Frind et al. (1985), simultaneously scale the recharge rates and the hydraulic conductivity. Such scaling does not change the structure of the flow simulated by their model. However, the hydraulic conductivity of the Borden aquifer is evaluated based on pumping and permeability tests. As such, it must be considered as an objective characteristic of the Borden aquifer. Scaling the hydraulic conductivity represents an ad hoc substitution of one geological object with another. Since the recharge pattern is not observable and is evaluated as an effective characteristic, it seems more natural to manipulate the recharge rates only. Frind and Hokkanen (1987) do not explain their reasons for scaling. Likely, they did this to satisfy the travel time to reach the furthest location to which the plume had spread, some 600–650 m from the down-gradient edge of the landfill. Proportional decreasing or increasing the recharge rates and the hydraulic conductivities affects the travel time.

At first sight, the Dupuit-Forchheimer model ignoring the vertical component of flow does not have tools for simulating curved, two-dimensional streamlines. Strack (1989) overcomes this controversy, suggesting that the incoming recharge pushes down the existing streamlines, curving them. He provides the mathematical expression describing the process. Gorokhovski and Weaver (2007), developing the D1_Flow model, applied his approach to one-dimensional flow in horizontally heterogeneous aquifers on an arbitrarily shaped base.

Let streamline S originate at location x_{st} on the water table (Fig. 4.5) and Q_S denotes the total flux $Q(x)$ at x_{st} [$Q_{\mathrm{S}} = Q(x_{\mathrm{st}})$]. Streamline S is the upper boundary of the Q_S part of the total flux $Q(x)$. Since the specific flux does not depend on depth according to the Dupuit-Forchheimer simplification, the following equality holds at any location $x \geq x_{\mathrm{st}}$:

$$\frac{Q(x)}{Q_S} = \frac{H(x) - Y(x)}{H_S(x) - Y(x)}. \tag{4.34}$$

It follows from Eq. 4.34 that

$$H(x) - Y(x) = \frac{Q(x)}{Q_S}(H_S(x) - Y(x)). \tag{4.35}$$

The travel time for a particle to reach location x moving along streamline S is

$$t(x) = R\theta \int_{s_{\mathrm{st}}}^{s_x} \frac{\mathrm{ds}}{v(s)}, \tag{4.36}$$

where R is the retardation factor, θ is the effective porosity, and $v(s)$ is the projection of the horizontal Darcy velocity $v(x)$ onto streamline S. (According to Frind and Hokkanen 1987, for the Borden aquifer, $\theta = 0.38$ and $R = 1$.) In a one-dimensional filtration model the Darcy velocity at any location x can be represented as

$$v(x) = \frac{Q_S}{H_S(x) - Y(x)}. \tag{4.37}$$

Table 4.4 Recharge patterns (cm/year) for evaluating streamlines and travel time

Interval (m)	0–140	140–300	300–600	600–800	800–1,050
Frind and Hokkanen (1987)	10	37	10	30	7
D1_Flow model:					
Best streamline	7	34	12.1	26.5	10
Best travel time	5.85	28.41	10.2	23	8.36

Correspondingly

$$v_S(x) = \frac{v(x)}{\sqrt{1 + \left(\frac{\mathrm{dH_S(x)}}{\mathrm{d}x}\right)^2}}. \tag{4.38}$$

Equation 4.36 can be rewritten as

$$t(x) = \frac{R\theta}{Q_S} \int\limits_{x_{\mathrm{st}}}^{x} (H_S(x) - Y(x)) \left(1 + \left(\frac{\mathrm{dH_S(x)}}{\mathrm{d}x}\right)^2\right) \mathrm{d}x. \tag{4.39}$$

The D1_Flow model integrates Eq. 4.39 numerically, using the trapezoid rule.

The D1_Flow model has been calibrated with respect to the upper boundary of the plume representing the streamline starting at the water table beneath the down-gradient edge of the landfill at $x = 300$ m. This streamline is the shortest and fastest way for contamination to spread. The goal of the calibration is to evaluate the recharge pattern for $x > 300$ m to provide the best reproduction of the streamline and the travel time for the plume to reach the furthest distance from the landfill, which is located somewhere in the interval 900−950 m. The starting point for calibrating is the recharge pattern accepted by Frind and Hokkanen (1987) (Table 4.4).

Calibration has been conducted in two steps. First, the recharge pattern providing the best reproduction of the streamline was found. The results are presented in Table 4.4 and Fig. 4.6. The magnitude of the errors in the best reproduction of the streamline by the D1_Flow model is equal to 5 cm. The second step is necessary as the travel time for the contaminant to reach $x = 900$ m with the obtained streamline and recharge rates is about 32 years instead of the expected 39–40 years. The recharge pattern providing travel time equal to 39.1 years to reach $x = 900$ m and 40.2 years to reach $x = 950$ m is presented in Table 4.3 also. The total flux Q_S under this streamline is 0.1253 m/day. This seems to be a satisfactory compromise between reproducing the shape of the streamline and the available travel time. The magnitude of the errors in reproducing the observed streamline is less than 5.04 cm. Some other streamlines obtained by Frind and Hokkanen (1987) and the D1_Flow model are shown in Fig. 4.7.

The calibration procedure has been simplified by the fact that, according to Eq. 4.34, the simulation results are defined by the ratio Q/Q_S. However, since the model is not an exact copy of the geological object and the procedure utilized in

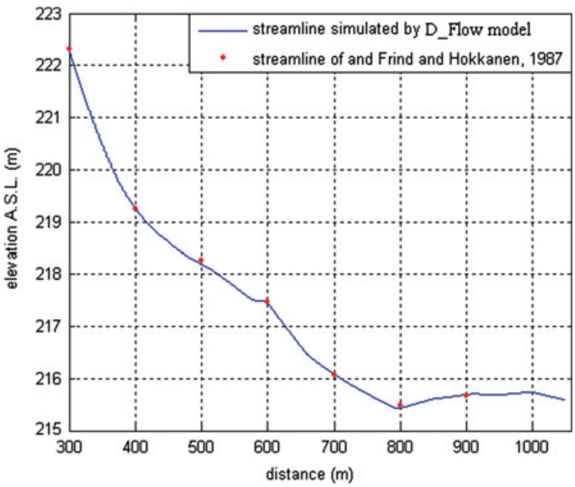

Fig. 4.6 Results of calibration of the D1_Flow model based on data of Frind and Hokkanen 1987, on the streamline starting at $x = 300$ m

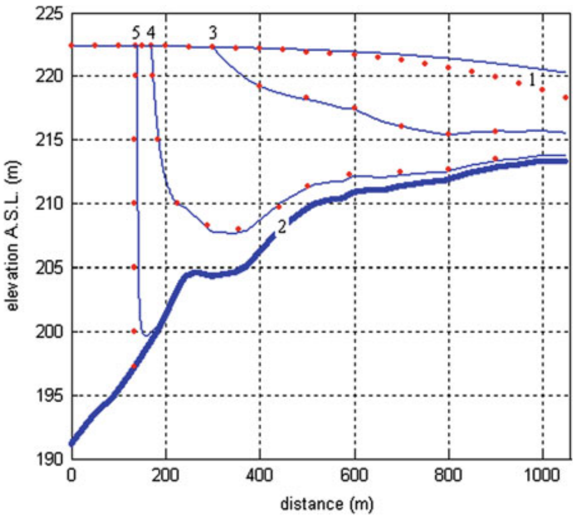

Fig. 4.7 Results of calibration of the D1_Flow model (*solid lines*) with respect to streamlines of Frind and Hokkanen (1987) (*dots*): *1*-water tables, *2*-base of aquifer, *3*-streamline starting at $x = 300$ m, *4*-streamline starting at $x = 170$ m, *5*-streamline starting at 140 m

the D1_Flow model is not more than an approximation of the real process, the final part of the second step required manual fitting of the simulation results to the observations. The manual fitting is not cumbersome either, as the D1_Flow model permits fitting with available data sequentially.

Summarizing, the simple D1_Flow model exploiting some obviously false assumptions yields results which are practically comparable to those yielded by the more physically sound model of Frind and Hokkanen (1987). In principle, models with larger number of governing parameters are more flexible, being easier to fit with available observations; for example, the D1_Flow model simulating the

Borden plume could reproduce the observations absolutely accurately, if the recharge rates changed at (and stayed constant between) the points of observations, but what does this prove? Thus, the quality of calibration, fitting the available observations, cannot be a decisive reason for choosing a model. (Compare with the chose of mathematical expressions depicting regional trends discussed in Sect. 3.1 and illustrated by Fig. 3.1).

The calibration of both models explicitly demonstrates the problem dependence of model identification. Indeed, Frind and Hokkanen (1987) scaled the recharge pattern and the hydraulic conductivities to satisfy the factual travel time. Their scaling leads to substitution of the empirically established properties of the object by different model parameters; that is, one object is substituted with another. In the case of the D1_Flow model, to achieve a good fit, only the recharge pattern was manipulated. The hydraulic conductivity, i.e., the hydrogeological object per se, remained the same. Nevertheless both calibrations can be considered as successful. However, the uncertainty of the simulation results in both cases cannot be evaluated in a provable way, since the simulations use many unverified and even incorrect assumptions, the most obvious of which are those about steady-state filtration plus the Dupuit-Forchheimer assumption in the case of the D1_Flow model.

Geological models are not exact copies of the real, not fully known, geological objects that they represent. Such models can be tuned to simulate satisfactorily the problems under conditions imposed in calibration. However, if the conditions change, parts of the objects that are unknown, not represented, or misrepresented can affect the objects' responses in ways that differ considerably from what is expected based on simulation models. Namely, this causes the problem dependence of model identification. (Inaccuracy of a mathematical model can produce similar effects which might be the subject of special research).

Model identification in hydrogeology is often considered as an inverse problem. This is not accurate. Model identification is an optimization problem usually. Its solution depends on the systems to be optimized. The systems include a number of factors: structures and properties of the objects, known and not known; the models representing them in the simulation; the mathematical descriptions of the processes in the model; actual and modeled boundary conditions; manmade and natural impacts affecting the available data; quality criteria for fitting the data; and monitoring networks used for evaluating the criteria (the list is not exhaustive). The optimal parameters are optimal, effective, in the sense they are assigned to be effective. However, if the system that they optimize is changed, those effective parameters may lose effectiveness and even become misleading. And this is indeed the case, since predictive problems differ from model identification problems in many respects.

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Chapter 5
Transformation of Geological Objects' Properties into Effective Model Parameters

One of the effects of the phenomenon of problem dependence of model identification is that the model parameters effective in a given formulation of the model identification may not be, and often are not, effective in the coupled predictive simulations. The reason is that the coupled predictive problem differs from the model identification problem in many respects. They can have different impacts, boundaries and boundary conditions, nature of simulating fields (water tables and streamlines, as in the example discussed in Sect. 4.4), quality criteria of simulation, and monitoring networks on which quality is evaluated. Even the mathematical models applied are often different (steady-state filtration in calibration versus transient in predictive simulations). The goal of model identification must be to provide the model parameters effective in predictive simulations, not just in calibration. The concept of transforming mechanisms introduced below is focused on providing the model parameters effective in predictive simulation.

5.1 Geological Objects and Simulation Models

As discussed in the previous chapters, to simulate underground flow and mass transport by solving differential equations describing the simulation processes within a site, we need to assign pertinent boundary conditions on the boundaries of the site of interest. Although some of the conditions can be controlled or induced by us, i.e., are known, a considerable part of them remains unknown but just assumed. To find the boundaries on which boundary conditions can be established, we usually have to go outside of the site of interest. If we cannot find them close enough to our site, then we consider that the boundaries are as if at infinity and, based on this assumption, evaluate the boundary conditions as close to the site as possible. Thus, simulation models must usually represent larger geological surroundings than the sites of interest.

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_5,

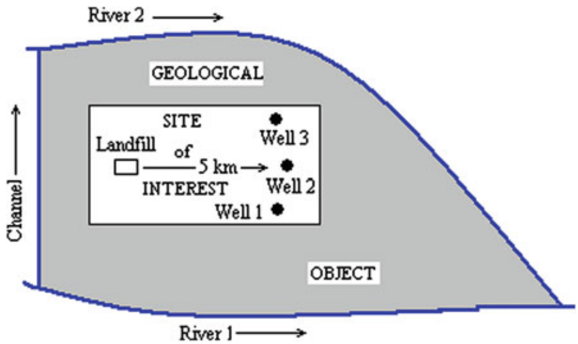

Fig. 5.1 Site of interest and geological object

Let us assume that the goal of simulation is to predict how construction of a landfill can affect water supplying wells (Fig. 5.1). Let rivers 1 and 2 and a channel be closely connected to the aquifer used for the water supply. This permits assignation of boundary conditions along those rivers and the channel and solving of the mass transport problem within the territory outlined by the rivers and the channel.

The territory including the sites of interest and outlined by the boundaries permitting assignation of boundary conditions required for solving pertinent hydrogeological and mass transport problems are called here *geological objects* (or just *objects*). Homogeneous geological units, the units comprising rocks and soils of the same lithological composition, origin, and geological history, are called *geological bodies* (or just *bodies*). Their properties are traditionally considered as constant. Space and time trends of the properties are rarely taking into account. However, when they are, the coefficients of the corresponding trends can be considered as properties of the geological bodies, constant within them.

Geological models (or just *models*) are simplified replicas of the geological objects. They introduce rules of interpolation and extrapolation of sparse available data on geological properties at every point of the objects, thereby filling the information gaps created by the paucity of the data. The interpretation rules are primitive. Models usually consist of homogeneous units called *model blocks* (or just *blocks*): One parameter value of each relevant property substitutes for the variety of that actual property's values within a given model block. This parameter and its value are called the *model block parameter* (or just*parameter*). Figure 5.2 illustrates the notions of the geological object and geological model. The object consists of five geological bodies, and the model of two blocks. If bodies 1.3 and 2.1 are actually the same geological body, they are considered as two different bodies, since they belong to different model blocks.

5.2 Transforming Mechanisms

Let an object comprise N geological bodies. Its geological model consists of M blocks ($M \leq N$). Block j represents N_j geological bodies with actual values of G of $(g_{j,1}, \ldots, g_{j,N_j})$, and model block parameter $\hat{g}_j$ substitutes for these values in

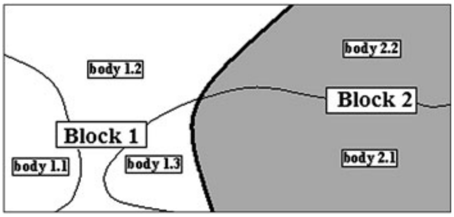

Fig. 5.2 Five-body geological structure and two-block model

predictive simulations. Conversion of actual property values of the geological bodies into the effective model block parameter is called *transformation*. The term is used to emphasize that the conversion is not necessarily statistical averaging, which is characterized by nonnegative weighting factors that sum to one.

Since geological models are not exact copies of the geological objects, the simulation results do not reproduce the objects' responses on natural and manmade impacts exactly. We can request only that the results be best in some predefined sense, i.e., satisfy some criterion of quality on a given monitoring network. The most popular and mathematically convenient is the least-squares criterion requiring minimization of the squared residuals between the data observed by the monitoring network and the corresponding simulation results. Other criteria can be applied as well. Model identification is the search for the set of model parameters providing the best, in a predefined sense, results of the pertinent predictive simulation, not just in calibration. Thus, the problem of model identification is an optimization problem.

The model which is best in a defined sense is called *effective*. The corresponding set of its parameters $(\hat{g}_1, \ldots, \hat{g}_j, \ldots, \hat{g}_M)$ is *effective*. Each parameter of the set is an *effective parameter*. A mathematical expression describing the transformation of actual values of property G of the geological bodies forming the geological object into the effective parameter $\hat{g}_j$, generalizing property G in block j, is called the *transforming mechanism* (or just the *mechanism*). The following equation represents one of the possible forms of such expressions:

$$\hat{g}_j = \sum_{m=1}^{M} \sum_{n=1}^{N_m} w_{j,m,n} g_{m,n}, \tag{5.1a}$$

where geological bodies are enumerated within each model block: $g_{m,n}$ is the actual value of property G in geological body n ($n = 1$ to N_m) belonging to model block m, and $w_{j,m,n}$ is the affecting factor describing the contribution of body n belonging to block m in forming the effective parameter value $\hat{g}_j$ of property G for block j. Equation 5.1a can be written also as

$$\hat{g}_j = \sum_{n=1}^{N} w_{j,n} g_n, \tag{5.1b}$$

where the enumeration of the geological bodies is total ($1 \leq n \leq N$) so g_n and $w_{j,n}$ are the actual value of property G in body n of the object. Block j for which the effective parameter value $\hat{g}_j$ is evaluated is called the *evaluated* block. Other blocks are called *affecting*.

Contrary to statistical averaging, which includes only bodies belonging to the evaluated block j, summations in Eq. 5.1 include all geological bodies of the geological object. Subsurface flow, as well as mass transport, is a dynamic process affected by the internal conditions on continuity of flow and hydraulic heads or water table elevations at the geological body contacts. The internal conditions bind all geologic bodies of the object in a united system, and the response occurring in a part of the object represented by some model block depends not only on properties of the bodies represented by this block but also on properties of each body of the object. Therefore, any transformation of a spatially variable property G related to modeling dynamic processes should incorporate relevant property values of all geological bodies.

Equation 5.1 represent a *linear transforming mechanism* if the affecting factors depend on positions of the geologic bodies and/or time only. If the affecting factors depend on geologic bodies' property values, Eq. 5.1 represents a *nonlinear transforming mechanism.*

The transforming mechanisms can be *property interrelated* also. The interrelation can reflect real bounds as in the cases of aquifer transmissivity (the product of aquifer thickness and hydraulic conductivity) and hydraulic diffusivity (the quotient of hydraulic transmissivity and storativity). The subsurface flow transport models are essentially governed by nondimensional coefficients, binding different physical parameters; for example, one-dimensional steady-state flow in a homogeneous aquifer is described by the equation

$$\frac{K\mathrm{d}\left(h(x)\frac{\mathrm{d}h(x)}{\mathrm{d}x}\right)}{\mathrm{d}x} = -N, \tag{5.2}$$

where $h(x)$ is the aquifer thickness, K is the hydraulic conductivity, and N is the recharge. Although Eq. 5.2 contains two parameters (K and N), it is actually governed by the dimensionless ratio $W = K/N$.

In the case of the interrelating mechanisms, the transforming mechanisms represented by Eq. 5.1b take the following form:

$$\hat{g}_{j,s} = \sum_{n=1}^{N}\sum_{p=1}^{P} w_{j,n,p}g_{n,p}, \tag{5.3}$$

where $\hat{g}_{j,s}$ is the effective value of property G_s in model block j, and $g_{n,p}$ is the actual value of property G_p of geological body n. The interrelating mechanisms are not discussed in this work, since it complicates presentation of the concept of the transforming mechanisms.

5.3 Properties of Transforming Mechanisms

Let a geological model be an exact replica of a geological object with respect to property G. This means that each model block is homogeneous in property G; i.e., all geological bodies represented by each block have the same value of property G. Thus, all bodies belonging to model block m have the same value g_m of property G. It is reasonable to assume in this case that the effective value $\hat{g}_j$ provided by Eq. 5.1a should be equal to the actual value of the property in block j:

$$\hat{g}_j = \sum_{m=1}^{M} \left(\sum_{n=1}^{N_m} w_{j,m,n} \right) g_m = g_j. \tag{5.4}$$

For Eq. 5.4 to be true for any set $\{g_m\}$ of actual property values, three obvious properties of the transforming mechanisms must hold.

Property 1 is expressed by the equality

$$\sum_{n=1}^{N_j} w_{j,j,n} = 1 \quad \text{for evaluated block } j; \tag{5.5}$$

that is, the affecting factors related to evaluated block j sum to one in any transforming mechanism forming effective parameter$\hat{g}_j$.

Property 2 is expressed by the equality

$$\sum_{n=1}^{N_m} w_{j,m,n} = 0 \quad \text{for affecting block } m \ (m \neq j); \tag{5.6}$$

that is, the affecting factors for any affecting block sum to zero. One more property follows from properties 1 and 2:

Property 3

$$\sum_{n=1}^{N} w_{j,n} = 1; \tag{5.7}$$

that is, the total sum of all affecting factors is equal to one.

The following example illustrates the above properties of the transforming mechanisms. Let a geological object comprise five geological bodies and its model consist of two blocks (Fig. 5.3). Two effective parameters ($\hat{g}_1$ and $\hat{g}_2$) must represent actual values of property G in simulations. Two transforming mechanisms convert properties of the geological bodies into the effective model parameters:

$$\begin{aligned} \hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4 + w_{1,5}g_5, \\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4 + w_{2,5}g_5, \end{aligned} \tag{5.8}$$

where $g_1 = g_{1,1}$, $g_2 = g_{1,2}$, $g_3 = g_{1,3}$, $g_4 = g_{2,1}$, and $g_5 = g_{2,2}$ in Fig. 5.3.

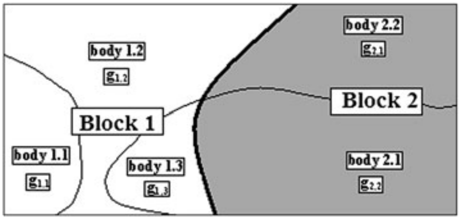

Fig. 5.3 Five-body object and two-block model

Properties of the transforming mechanisms can be easily demonstrated by mechanisms 5.8. Indeed, let the discussed model be an exact replica of the object. This means that property G is the same within each model block:

$$g_1 = g_2 = g_3 = G_1 \quad \text{and} \quad g_4 = g_5 = G_2. \tag{5.9}$$

Then, Eq. 5.8 converts into equations

$$\begin{aligned} \hat{g}_1 &= (w_{1,1} + w_{1,2} + w_{1,3})G_1 + (w_{1,4} + w_{1,5})G_2, \\ \hat{g}_2 &= (w_{2,1} + w_{2,2} + w_{2,3})G_1 + (w_{2,4} + w_{2,5})G_2. \end{aligned} \tag{5.10}$$

For the model which is an exact replica of an object, the model block effective parameters are equal to the actual property values:

$$\begin{aligned} \hat{g}_1 &= (w_{1,1} + w_{1,2} + w_{1,3})g_1 + (w_{1,4} + w_{1,5})g_2 = G_1, \\ \hat{g}_2 &= (w_{2,1} + w_{2,2} + w_{2,3})g_1 + (w_{2,4} + w_{2,5})g_2 = G_2. \end{aligned} \tag{5.11}$$

Equalities 5.11 must hold for any values G_1 and G_2. To make this possible, mechanisms 5.11 should have properties 1 and 2:

$$\begin{aligned} &w_{1,1} + w_{1,2} + w_{1,3} = 1 && \text{Property 1} \\ &w_{1,4} + w_{1,5} = 0 && \text{Property 2} \\ &w_{2,1} + w_{2,2} + w_{2,3} = 0 && \text{Property 2} \\ &w_{2,4} + w_{2,5} = 1 && \text{Property 1} \end{aligned}$$

It follows from property 2 that, if an affecting block represents more than one geological body, at least one of affecting factors of the block is negative. This means that, in general, the effective parameters of models are not of the statistical nature. That is, they are not statistical averages with nonnegative weighting factors summing to one. In the case of homogeneous models, due to property 1, the effective parameters can be the statistical averages. However, as shown in Chap. 7, summing of the affecting factors of the evaluated blocks to one does not warrant that all the factors are not negative. The fact that all geological bodies of the object participate in forming effective parameters for any block undermines the statistical nature of the effective parameters also.

The effective parameters are the characteristics optimizing the system made up by the geological structure of the object, the model representing it, the boundary conditions, the natural or manmade impact which is to be simulated, the criterion of quality of planning predictive simulations, and the monitoring network on which the given criterion is evaluated. The system changes if any of the above listed factors change, and this changes the transforming mechanisms. Even the progress of time can change the transforming mechanisms and the effective parameter values. (See examples in Chaps. 6 and 7).

The presence of negative affecting factors in the transforming mechanisms can lead to physically incorrect values of the effective parameters such as negative hydraulic conductivities and transmissivities (see Chaps. 6–8 for examples). This emphasizes that the effective parameters are deprived of physical meaning. They are system characteristics providing the system efficiency and nothing more. To be effective in a changed system, different effective parameters and different transforming mechanisms are required (showing problem dependence at work).

A physically incorrect effective parameter is self-obvious. However, the effective parameters, being correct physically, may be incorrect geologically, exceeding the range of the actual values of the property they represent. Geological incorrectness is not obvious. Geologically incorrect effective parameters, being effective in a given predictive problem formulation, may become misleading and even dangerous in other applications.

Problem dependence is usually seen as an obstacle or, at least, as a nuisance. On the other hand, the problem dependence of the effective parameters permits different values of the effective parameters to be obtained, using different model identification problem formulations. This permits better understanding of the structures of geological objects and can be used for formulating and solving inverse hydrogeological problems (Chap. 9).

The transforming mechanisms, defined by their affecting factors, describe contributions of different objects' parts to the effective parameters of the simulation models. Therefore, being evaluated before starting field investigations (Chap. 8), they can be a tool for their optimization. The transforming mechanisms can be applied also for assigning monitoring networks and even simulation models.

Transforming mechanisms are introduced here in the hydrogeological context. However, their introduction does not assume any hydrogeological specificity. It would not be surprising if such mechanisms with analogous properties are known to professionals in the field of optimization. In any case, the transforming mechanisms and their properties can be applied to other fields where simplified versions of complex systems are in use, such as geophysics, engineering geology, and environmental sciences.

Chapter 6
Examples of Linear Transforming Mechanisms

6.1 One-Dimensional Steady-State Filtration to Fully Penetrating Trench

Let us consider one-dimensional steady-state underground flow in an unconfined aquifer on a horizontal base with constant recharge N to a fully penetrating trench at $X_0 = 0$ (Fig. 6.1). The aquifer is piecewise homogeneous. Its hydraulic conductivity changes at locations X_1, X_2, and X_3, taking within the intervals $[X_0, X_1]$, $(X_1, X_2]$, $(X_2, X_3]$, and $(X_3, X_4]$ the values K_1, K_2, K_3, and K_4. Recharge $N = 0.0001$ m/day, and $X_1 = 25$, $X_2 = 50$, $X_3 = 75$, and $X_4 = 100$ m. The outer boundary conditions are given as the aquifer thickness h_0 at X_0 and the slope (gradient) of the water table at X_4:

$$h_0 = h(X_0), \quad \frac{\mathrm{d}h}{\mathrm{d}x}|_{x=X_4} = 0.$$

Within homogeneous interval j, $[X_{j-1}, X_j]$, the flow is described by the equation

$$\frac{\mathrm{d}\left(K_j\left(h(x)\,\frac{\mathrm{d}h(x)}{\mathrm{d}x}\right)\right)}{\mathrm{d}x} = -N, \quad X_{j-1} \le x \le X_j, \tag{6.1}$$

where $h(x)$ is the aquifer thickness at x.

The inner boundary conditions on continuity of the water table elevation and the flux at locations $X_1 = 25$, $X_2 = 50$, and $X_3 = 75$ m are

$$\begin{aligned} \lim_{x\to X_j}(h(x)) &= \lim_{X_j \leftarrow x}(h(x)) \\ K_j\left(h\frac{\mathrm{d}h}{\mathrm{d}x}\right)\Bigg|_{x\to X_j} &= K_{j+1}\left(h\frac{\mathrm{d}h}{\mathrm{d}x}\right)\Bigg|_{X_j \leftarrow x}. \end{aligned} \tag{6.2}$$

Integrating Eq. 6.1, using the outer and inner boundary conditions for interval $[X_{j-1}, X_j]$, yields (see the inference in Text Box 6.1):

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_6,

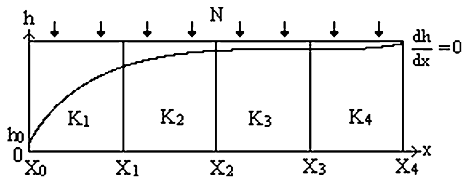

Fig. 6.1 One-dimensional steady-state flow to a fully penetrating trench in an unconfined aquifer

$$h^2(x) = h_{j-1}^2 + 2\frac{N}{K_j}(L - X_{j-1})(x - X_{j-1}) - \frac{N}{K_j}(x - X_{j-1})^2, \quad X_{j-1} \le x \le X_j. \tag{6.3}$$

> Text Box 6.1
>
> Integrating Eq. 6.1 with the outer and inner boundary condition yields the general solution
>
> $$h^2(x) = -\frac{N}{K}(x - X_{j-1})^2 + C_1(x - X_{j-1}) + C_2, \quad X_{j-1} \le x \le X_j,$$
>
> where C_1 and C_2 are arbitrary constants. To obtain the particular solution of our problem, we need to find C_1 and C_2 based on the boundary conditions at the ends of intervals at locations: $X_0 = 25$, $X_1 = 25$, $X_2 = 50$, $X_3 = 75$, and $X_4 = L = 75$ m. It follows immediately from the fist condition (6.2) that $C_2 = h_{j-1} = h(X_{j-1})$. To find C_1, we have to write the equation for flux at the same location:
>
> $$2K\left(h(x)\frac{\mathrm{d}h(x)}{\mathrm{d}x}\right) = 2N(L - x) = -2N(x - X_{j-1}) + C_1.$$
>
> So, $C_1 = 2N(L - X_{j-1})$, and the particular solution, Eq. 6.3, follows

The squared thickness of the aquifer $h_{j\,=\,1,\ldots4}$ observed at locations X_1, X_2, X_3, and X_4 follows from Eq. 6.3 as

$$h_j^2 = h_{j-1}^2 + \frac{N}{K_j}(2L - X_{j-1} - X_j)(X_j - X_{j-1}). \tag{6.4}$$

Let the simulation geological model consist of two homogeneous blocks with the boundary between them at location $X = 50$ m. The goal is to evaluate two effective hydraulic conductivities, $\hat{K}_1$ and $\hat{K}_2$, for the model blocks based on observations on the thicknesses of the aquifer at locations $X_1 = 25$, $X_2 = 50$, $X_3 = 75$, and $X_4 = 100$ m, selected to simplify calculations. The simulated thickness of the aquifer at those locations can be calculated as

$$\hat{h}_j^2 = \hat{h}_{j-1}^2 + \frac{N}{\hat{K}_i}(2X_4 - X_j - X_{j-1})(X_j - X_{j-1}), \quad i = 1,\ 2;\ j = 1,\ 2,\ 3,\ 4. \tag{6.5}$$

(The effective hydraulic conductivity $\hat{K}_1$ substitutes for K_1 and K_2, and $\hat{K}_2$ for K_3 and K_4). The goodness of fit for the parameters $\hat{K}_1$ and $\hat{K}_2$ is evaluated by the criterion

$$s = \sum_{j=1}^{4} p_j \left(\hat{h}_j^2 - h_j^2 \right)^2, \tag{6.6}$$

in which the weight p_j assigns the significance of the squared differences between the observed and simulation results at location X_j (p_j may be any number, including negative ones). If all observations are equally important, all weights p_j must be equal, say to 1, to 2, or 52. If, for example, the accuracy of simulations must increase with distance, the weights can be assigned as $p_1 = 1$, $p_2 = 2$, $p_3 = 3$, and $p_4 = 4$, or $p_1 = 3$, $p_2 = 7$, $p_3 = 8$, and $p_4 = 12$, and so on.

Substituting in Eq. 6.4 the given values of $X_0 = 0$, $X_1 = 25$, $X_2 = 50$, $X_3 = 75$, $X_4 = 100$ m, and $N = 0.0001$ m/day yields

$$\begin{aligned} h_1^2 &= h_0^2 + 0.4375 g_1, \\ h_2^2 &= h_0^2 + 0.4375 g_1 + 0.3125 g_2, \\ h_3^2 &= h_0^2 + 0.4375 g_1 + 0.3125 g_2 + 0.1875 g_3, \\ h_4^2 &= h_0^2 + 0.4375 g_1 + 0.3125 g_2 + 0.1875 g_3 + 0.0625 g_4. \end{aligned} \tag{6.7}$$

The same procedure for Eq. 6.5 for simulation results yields

$$\begin{aligned} \hat{h}_1^2 &= h_0^2 + 0.4375 \hat{g}_1, \\ \hat{h}_2^2 &= h_0^2 + 0.75 \hat{g}_1, \\ \hat{h}_3^2 &= h_0^2 + 0.75 \hat{g}_1 + 0.1875 \hat{g}_2, \\ \hat{h}_4^2 &= h_0^2 + 0.75 \hat{g}_1 + 0.25 \hat{g}_2, \end{aligned} \tag{6.8}$$

where $g_1 = 1/K_1$, $g_2 = 1/K_2$, $g_3 = 1/K_3$, $g_4 = 1/K_4$ are called the actual hydraulic resistivity, and $\hat{g}_1 = 1/\hat{K}_1$ and $\hat{g}_2 = 1/\hat{K}_2$ are the effective hydraulic resistivities.

Substituting the simulation results Eq. 6.8 in criterion (6.6) yields

$$\begin{aligned} s = p_1 \left(h_0^2 + 0.4375 \hat{g}_1 - h_1^2 \right)^2 + p_2 \left(h_0^2 + 0.75 \hat{g}_1 - h_2^2 \right)^2 \\ + p_3 \left(h_0^2 + 0.75 \hat{g}_1 + 0.1875 \hat{g}_2 - h_3^2 \right)^2 + p_4 \left(h_0^2 + 0.75 \hat{g}_1 + 0.25 \hat{g}_2 - h_4^2 \right)^2. \end{aligned} \tag{6.9}$$

Application of the standard procedure of the least-squares method to the sum (6.9) leads to the following linear system of equations for calculating the effective values $\hat{g}_1$ and $\hat{g}_2$ based on the observed differences $\left(h_i^2 - h_0^2 \right)$ $(i = 1, 2, 3, 4)$:

$$\begin{aligned} &(0.4375^2 p_1 + 0.75^2 (p_2 + p_3 + p_4)) \hat{g}_1 + 0.75(0.1875 p_3 + 0.25 p_4) \hat{g}_2 \\ &\quad = 0.4375 p_1 \left(h_1^2 - h_0^2 \right) + 0.75 \left(p_2 \left(h_2^2 - h_0^2 \right) + p_3 \left(h_3^2 - h_0^2 \right) + p_4 \left(h_4^2 - h_0^2 \right) \right) \\ &0.75(0.1875 p_3 + 0.25 p_4) \hat{g}_1 + (0.1875^2 p_3 + 0.25^2 p_4) \hat{g}_2 \\ &\quad = 0.1875 p_3 \left(h_3^2 - h_0^2 \right) + 0.25 p_4 \left(h_4^2 - h_0^2 \right). \end{aligned} \tag{6.10}$$

Matrix c of system (6.10) is

$$c = \begin{Bmatrix} 0.4375^2 p_1 + 0.75^2(p_2 + p_3 + p_4) & 0.75(0.1875p_3 + 0.25p_4) \\ 0.75(0.1875p_3 + 0.25p_4) & 0.1875^2 p_3 + 0.25^2 p_4 \end{Bmatrix} \quad (6.11a)$$

It depends on the structure of the object and simulation model, the observation network, and the weights, but not on the observations. The right-hand terms (vector b) of system (6.10)

$$b = \begin{Bmatrix} 0.4375p_1\left(h_1^2 - h_0^2\right) + 0.75\left(p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right)\right) \\ 0.1875p_3\left(h_3^2 - h_0^2\right) + 0.25p_4\left(h_4^2 - h_0^2\right) \end{Bmatrix} \quad (6.11b)$$

depend on observations.

The effective hydraulic resistivities are solution of system (6.10)

$$\hat{g}_1 = \Delta_1/\Delta, \quad \hat{g}_2 = \Delta_2/\Delta \quad (6.12a)$$

with determinants

$$\begin{aligned} \Delta &= c_{11}c_{22} - c_{12}c_{21}, \\ \Delta_1 &= b_1c_{22} - b_2c_{12}, \\ \Delta_2 &= b_2c_{11} - b_1c_{21}. \end{aligned} \quad (6.12b)$$

Expression (6.12) solves the above-formulated model identification problem. To find the mechanisms transforming the actual hydraulic resistivities g_1, g_2, g_3, and g_4 into the effective resistivities $\hat{g}_1$ and $\hat{g}_2$, it is necessary to express vector b (6.11b) and solution 6.12a in terms of the resistivities g_1, g_2, g_3, and g_4. This procedure yields

$$\begin{aligned} b_1 &= 0.4375\,(0.4375p_1 + 0.75(p_2 + p_3 + p_4))g_1 + 0.3125 \times 0.75\,(p_2 + p_3 + p_4)g_2 \\ &\quad + 0.1875 \times 0.75(p_3 + p_4)g_3 + 0.75 \times 0.0625p_4g_4, \\ b_2 &= 0.4375\,(0.1875p_3 + 0.25\,p_4)g_1 + 0.3125\,(0.1875p_3 + 0.25p_4)g_2 \\ &\quad + 0.1875\,(0.1875p_3 + 0.25p_4)g_3 + 0.25 \times 0.0625p_4g_4. \end{aligned} \quad (6.13)$$

Let us introduce vectors W_1 and W_2 constituted by the multipliers of the hydraulic resistivities g_1, g_2, g_3, and g_4 in Eq. 6.13:

$$W_1 = \begin{Bmatrix} 0.4375\,(0.4375p_1 + 0.75\,(p_2 + p_3 + p_4)) \\ 0.3125 \times 0.75\,(p_2 + p_3 + p_4) \\ 0.1875 \times 0.75(p_3 + p_4) \\ 0.75 \times 0.0625p_4 \end{Bmatrix}$$

$$W_2 = \begin{Bmatrix} 0.4375\,(0.1875p_3 + 0.25p_4) \\ 0.3125\,(0.1875p_3 + 0.25p_4) \\ 0.1875\,(0.1875p_3 + 0.25p_4) \\ 0.25 \times 0.0625p_4 \end{Bmatrix} \quad (6.14)$$

Table 6.1 Cases 6.2.1 and 6.2.2: distributions of the hydraulic conductivity values

Intervals (m)	0–25	25–50	50–75	75–100
Hydraulic conductivity (m/day)	K_1	K_2	K_3	K_4
Case 6.2.1	1	0.9	0.2	0.1
Case 6.2.2	0.1	0.2	0.9	1

Table 6.2 Case 6.2.1: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1 = 1.0011$		$\hat{K}_2 = 0.1678$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	0.4475	0.7947	1.7322	2.3572
Squared simulated aquifer thickness (m^2)	0.4470	0.7592	1.8766	2.2491

Then, the affecting factors of the pertinent transforming mechanisms can be calculated as

$$\begin{aligned} \{w_{11}, w_{12}, w_{13}, w_{14}\} &= \left\{ \frac{W_1 c_{22} - W_2 c_{21}}{c_{11} c_{22} - c_{12} c_{21}} \right\}', \\ \{w_{21}, w_{22}, w_{23}, w_{24}\} &= \left\{ \frac{W_2 c_{11} - W_1 c_{12}}{c_{11} c_{22} - c_{12} c_{21}} \right\}'. \end{aligned} \tag{6.15}$$

6.2 Illustrative Cases

Several cases are presented in this section to get a better feeling for the transforming mechanisms, their properties, and their sensitivity to each element of the model identification problem formulation.

Cases 6.2.1 and 6.2.2 These cases differ only with respect to the distributions of the actual hydraulic conductivity values (Table 6.1). The weighting is uniform (all weights are equal to one). The values of the effective hydraulic resistivities for model blocks 1 (interval [0, 50 m]) and 2 (interval [50, 100 m]) are evaluated, using the transforming mechanisms, the affecting factors, calculated by expression (6.15). Since those are linear transforming mechanisms, the affecting factors do not depend on the hydraulic conductivity distributions and are the same for both cases:

$$\begin{aligned} \hat{g}_1 &= 0.6861 g_1 + 0.3139 g_2 + 0.0072 g_3 - 0.0072 g_4, \\ \hat{g}_2 &= -0.3451 g_1 + 0.3451 g_2 + 0.8155 g_3 + 0.1845 g_4. \end{aligned} \tag{6.16}$$

The results for case 6.2.1 are presented in Table 6.2 and Fig. 6.2. They seem to be satisfying. The maximal error in the aquifer thickness is 0.0538 m at $x = 75$ m.

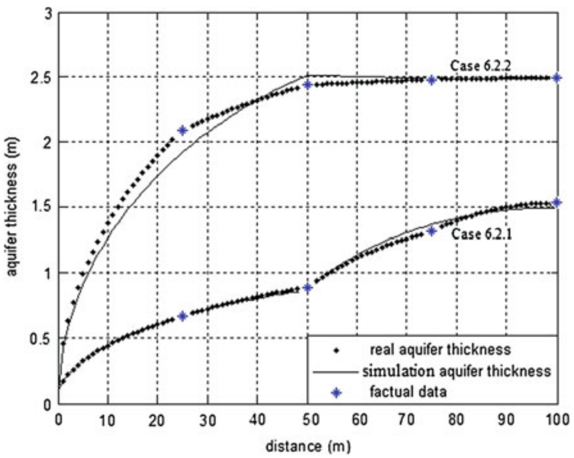

Fig. 6.2 Cases 6.2.1 and 6.2.2: comparison of factual and simulated aquifer thicknesses

Table 6.3 Case 6.2.2: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1 = 0.1186$		$\hat{K}_2 = -1.5751$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	3.6987	6.3335	6.2144	6.1748

The results of case 6.2.2 are presented in Fig. 6.2 and Table 6.3. They are not so good, compared with the result of case 6.2.1, with maximal error in the aquifer thickness equal to 0.1708 m at $x = 25$ m. The most disappointing is the negative value of the effective hydraulic conductivity $\hat{K}_2$, which is meaningless physically.

The first urge is to disregard case 6.2.2 as an incorrect formulation of the model identification problem, but what is wrong with the formulation? It does not differ from that of case 6.2.1. The transforming mechanisms are the same. The effective hydraulic resistivities are unique solutions of linear systems which are stable. What is more important, being physically incorrect, they provide the effective simulation of the water table or the thickness of the aquifer at the observation locations, doing exactly what was required of them. Sure, it would be wrong to apply these hydraulic conductivities to reproducing streamlines, but the streamlines were not the goal of the optimization.

The negative conductivity appeared as compensation for a very steep growth of the aquifer thickness near the trench and its very slow growth at the right half of the object, that is, as a consequence of the applied optimization procedure. By the way, the value of the effective conductivity $\hat{K}_1$ in case 6.2.1 is slightly greater than the real-world hydraulic conductivity K_1. Thus, although correct physically, it is incorrect geologically. In the following cases, this phenomenon demonstrates itself more clearly.

Table 6.4 Case 6.2.3: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1 = 0.0667$		$\hat{K}_2 = 0.4737$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	6.5725	11.2600	11.6558	11.7878

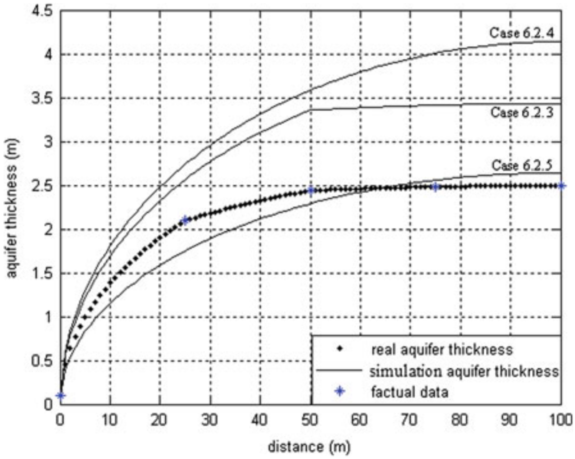

Fig. 6.3 Cases 6.2.3, 6.2.4, and 6.2.5: comparison of factual and simulated aquifer thickness

To avoid the use of the negative value of the effective hydraulic conductivity $\hat{K}_2$ in case 6.2.2, let us try more physically appropriate model parameters: the harmonic means of the actual hydraulic conductivities.

Case 6.2.3 The effective hydraulic conductivity of the above two blocks is assigned as harmonic means:

$$\hat{K}_1 = \frac{K_1 K_2}{K_1 + K_2} = \frac{0.1 \times 0.2}{0.1 + 0.2} = 0.0667 \text{ m/day},$$
$$\hat{K}_2 = \frac{K_3 K_4}{K_3 + K_4} = \frac{0.9 \times 1}{1.9} = 0.4737 \text{ m/day}.$$

Substituting these values of the hydraulic conductivities into Eq. 6.8 yields the results presented in Table 6.4 and Fig. 6.3. The advantage of the formulation of the model identification problem in case 6.2.2 is obvious. (Note that the above values of the model parameters are not geologically correct).

Case 6.2.4 Let us try a homogeneous (one-block) simulation model with the effective hydraulic conductivity assigned as the harmonic mean of the four factual values of hydraulic conductivity:

$$\hat{K} = \frac{1}{\frac{1}{K_1} + \frac{1}{K_2} + \frac{1}{K_3} + \frac{1}{K_4}} = \frac{1}{\frac{1}{0.1} + \frac{1}{0.2} + \frac{1}{0.9} + \frac{1}{1}} = 0.0584 \,\text{m/day}.$$

Table 6.5 Case 6.2.4: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K} = 0.0584$			
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	7.4961	12.8433	16.0517	17.1211

Table 6.6 Case 6.2.5: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K} = 0.1436$			
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	3.0572	5.2338	6.5397	6.9750

The results of case 6.2.4 are presented in Table 6.5 and Fig. 6.3. Note that the above statistics is geologically incorrect again.

Comparison of the results of cases 6.2.2, 6.2.3, and 6.2.4 demonstrates that the physically incorrect effective parameters perform better, much better, than those assigned from physical and statistical consideration. Besides the latter are geologically incorrect as well. So, it is up to the modeler to decide what the model parameters are preferable, i.e., simulating results more accurately or yielding less accurate but 'politically correct' results. (Political correctness is mentioned here based on the author experience: each time when the efficiency of the physically incorrect parameters was demonstrated, hydrogeologists object to them just because of their physical incorrectness.)

Case 6.2.5 It is interesting also to compare cases 6.2.3 and 6.2.4 with the homogeneous (one-block) model optimized in the sense of criterion (6.6) with uniform weighting ($p_j = 1, j = 1, 2, 3, 4$). The corresponding effective hydraulic resistivity in this case is equal to

$$\hat{g} = \frac{0.4375\left(h_1^2 - h_0^2\right) + 0.75\left(h_2^2 - h_0^2\right) + 0.9375\left(h_3^2 - h_0^2\right) + \left(h_4^2 - h_0^2\right)}{0.4375^2 + 0.75^2 + 0.9375^2 + 1}. \quad (6.17)$$

The corresponding transforming mechanism can be obtained by substituting into the equations the values of the differences $\left(h_j^2 - h_0^2\right)$ from Eq. 6.7

$$\hat{g} = 0.5193 g_1 + 0.3190 g_2 + 0.1380 g_3 + 0.0237 g_4. \quad (6.18)$$

The results of case 6.2.5 are presented in Fig. 6.3 and Table 6.6. Although they are worse than the ones in case 6.2.2, they are considerably better than those of cases 6.2.3 and 6.2.4.

Table 6.7 Case 6.2.6: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.1219$		$\hat{K}_2 = 7.0757$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	3.5997	6.1637	6.1902	6.1990

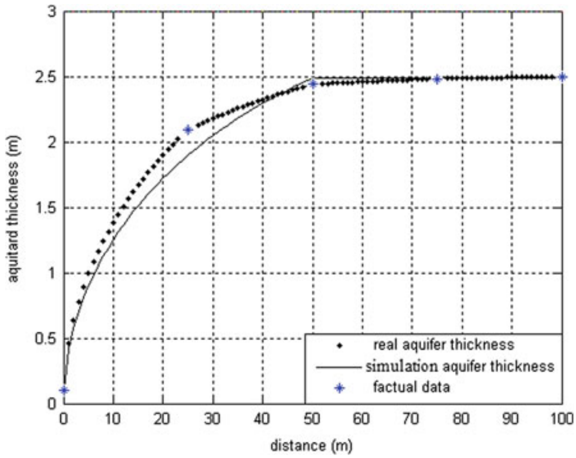

Fig. 6.4 Case 6.2.6: comparison of factual and simulated aquifer thickness

Case 6.2.6 If, for any reason, we are not satisfied with the results yielded by formulations of the problem identification in case 6.2.2, we can try different ones; for example, we can assign weights increasing with distance from the trench, say, $p_1 = 1, p_2 = 2, p_3 = 3$, and $p_4 = 4$. Corresponding transforming mechanisms are

$$\begin{aligned} \hat{g}_1 &= 0.6407g_1 + 0.3593g_2 + 0.0133g_3 - 0.0133g_4, \\ \hat{g}_2 &= -0.1891g_1 + 0.1891g_2 + 0.7802g_3 + 0.2198g_4. \end{aligned} \quad (6.19)$$

The results of case 6.2.6 are presented in Table 6.7 and Fig. 6.4. The maximal error in the aquifer thickness is 0.2160 m at $x = 25$ m. Although the maximal error is slightly greater than in case 6.2.2 (0.1708 m), the accuracy of the results in case 6.2.6 grows with distance due to the choice of the weights. Moreover, the effective conductivity $\hat{K}_2$ is physically correct, being positive. However, it is incorrect geologically, exceeding the actual hydraulic conductivity K_3 and K_4 considerably. This can make the model as erroneous as the physically incorrect effective value $\hat{K}_2$ in case 6.2.2 and in some different formulations of the simulation problem.

Case 6.2.7 Let us change the observation network. We come back to the uniform weighting, but move the observation from location $x = 25$ m to $x = 10$ m. This

Table 6.8 Case 6.2.7: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.1244$		$\hat{K}_2 = 1.4642$	
Monitoring location (m)	10	50	75	100
Squared factual aquifer thickness (m^2)	1.9100	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	1.5373	6.0389	6.1669	6.2096

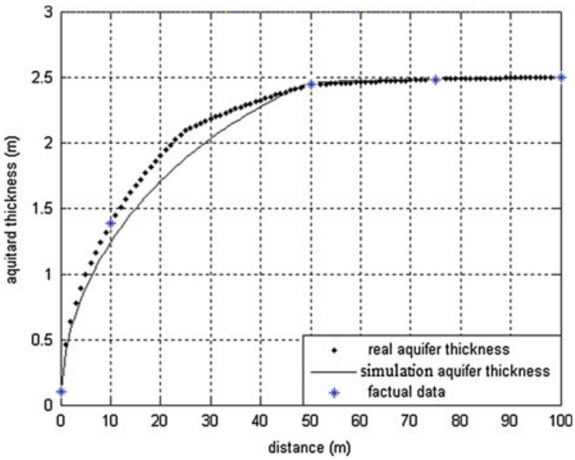

Fig. 6.5 Case 6.2.7: comparison of factual and simulated aquifer thickness

leads to changing the above system composed by the geological object, simulation model, and observation network. In turn, this leads to a different system of equations for finding the effective conductivities and the transforming mechanisms. The effective hydraulic resistivities $\hat{g}_1$ and $\hat{g}_2$ correspondingly are solutions of system:

$$\begin{aligned}
&(0.19^2 p_1 + 0.75^2(p_2 + p_3 + p_4))\hat{g}_1 + 0.75(0.1875 p_3 + 0.25 p_4)\hat{g}_2 \\
&\qquad = 0.19 p_1\left(h_1^2 - h_0^2\right) + 0.75\left(p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right)\right), \\
&0.75\,(0.1875 p_3 + 0.25 p_4)\hat{g}_1 + (0.1875^2 p_3 + 0.25^2 p_4)\,\hat{g}_2 \\
&\qquad = 0.1875 p_3\left(h_3^2 - h_0^2\right) + 0.25 p_4\left(h_4^2 - h_0^2\right).
\end{aligned} \tag{6.20}$$

The corresponding transforming mechanisms are

$$\begin{aligned}
\hat{g}_1 &= 0.6076 g_1 + 0.3924 g_2 + 0.0091 g_3 - 0.0091 g_4, \\
\hat{g}_2 &= -0.0814 g_1 + 0.0814 g_2 + 0.8096 g_3 + 0.1904 g_4.
\end{aligned} \tag{6.21}$$

The results of case 6.2.7 are presented in Table 6.8 and Fig. 6.5. The maximal error in the aquifer thickness is 0.1968 m at $x = 25$ m.

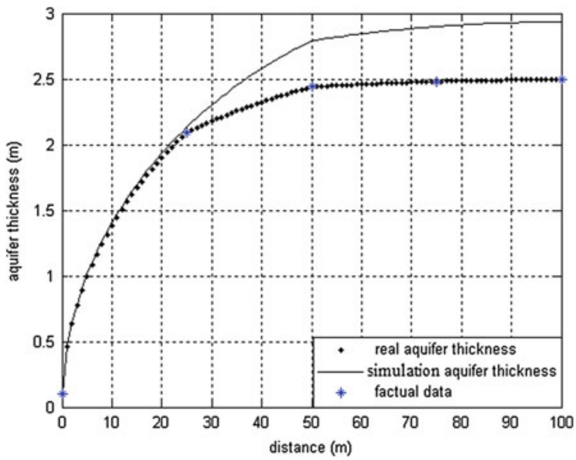

Fig. 6.6 Case 6.2.8: comparison of factual and simulated aquifer thickness

Table 6.9 Case 6.2.8: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.0964$		$\hat{K}_2 = 0.3043$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulated aquifer thickness (m^2)	4.5472	7.7881	8.4041	8.6095

It is worth noting that the model identification in case 6.2.7 is also geologically incorrect: the effective hydraulic $\hat{K}_2$ exceeds the factual values of the hydraulic conductivity.

Case 6.2.8 Let us consider one more alternative to the model identification problem presented in case 6.2.2. This time we change the model itself: the first block of the new model coincides with the first geological body (interval [0, 25 m]). The second block (interval [25, 100 m]) consists of three geological bodies. The observation network and weights are the same as in case 6.2.2. The system of equations for finding the effective values $\hat{g}_1$ and $\hat{g}_2$ is

$$\begin{aligned} &0.4375(p_1 + p_2 + p_3 + p_4)\hat{g}_1 + (0.3125p_2 + 0.5p_3 + 0.5625p_4)\hat{g}_2 \\ &\quad = p_1\left(h_1^2 - h_0^2\right) + p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right), \\ &0.4375(0.3125p_2 + 0.5p_3 + 0.5625p_4)\hat{g}_1 + \left(0.3125^2p_2 + 0.5^2p_3 + 0.5625^2p_4\right)\hat{g}_2 \\ &\quad = 0.3125p_2\left(h_2^2 - h_0^2\right) + 0.5p_3\left(h_3^2 - h_0^2\right) + 0.5625p_4\left(h_4^2 - h_0^2\right). \end{aligned} \tag{6.22}$$

The transforming mechanisms in this case are

$$\begin{aligned}\hat{g}_1 &= 1 \times g_1 + 0.0948 g_2 - 0.0743 g_3 - 0.0205 g_4,\\ \hat{g}_2 &= 0 \times g_1 + 0.5612 g_2 + 0.3673 g_3 + 0.0715 g_4.\end{aligned} \tag{6.23}$$

The results of case 6.2.8 are presented in Fig. 6.6 and Table 6.9. The maximal error in the aquifer thickness is 0.4405 m at $x = 100$ m. In general, the results are considerably worse than those in case 6.2.2. The effective parameters are incorrect geologically. However, the accuracy of reproducing the aquifer thickness in the interval [0, 25 m] is impressive. Maybe, it is worth contemplating application of different models to different parts of geological objects.

6.3 Discussion on Illustrative Cases

Table 6.10 summarizes the results of Sect. 6.2. The cases clearly demonstrate the problem dependence of model identification and support the statement that "it is not possible to define a consistent effective parameter value to reproduce the response of a spatially variable pattern of parameter values" (Beven 1989). We see that the effective parameters of predictive models and the transforming mechanisms depend on geological conditions (cases 6.2.1 and 6.2.2), and literally on each element of the simulation problem formulation (cases 6.2.2, 6.2.5–6.2.8). All transforming mechanisms have properties 1–3, and they are not statistics, besides the transforming mechanism presented by Eq. 6.18.

The problems in Sect. 6.2 are linear with respect to the squared thickness of the aquifer. Therefore, they do not support the most popular explanation of the phenomenon of problem dependence as due to nonlinearity of the simulation processes. Being results of optimization, the effective parameters are not physical or geological entities. They are characteristics of the system made up not only by geological objects but also by all elements of the model identification problem formulations. This is why the effective parameters can be incorrect physically and geologically, but still remain effective in pertinent optimizations. However, they can become misleading, if predictive simulations deal with systems different from those in which they are obtained as effective. Case 6.2.2 is revealing in this sense. The effective hydraulic conductivities $\hat{K}_1 = 0.1186$ and $\hat{K}_2 = -1.5751\,\mathrm{m/day}$ satisfactorily reproduce the aquifer thickness but are misleading in evaluations of streamlines, which are not a subject of optimization in the calibration.

At earlier stages of investigation, exact formulations of simulation problems may not be known yet. Then the goal of model identification is to find geologically correct parameters; i.e., the model characteristics must be within the range of factual properties of the geological object of interest. The transforming mechanism, as in case 6.2.5, being averaging of statistical nature, can serve this end. However, to be sure that the effective parameter values are indeed averaging of statistical nature, the transforming mechanisms must be presented explicitly.

Table 6.10 Transforming mechanisms and effective resistivities $\hat{G}$ (day/m) and hydraulic conductivities $\hat{K} = 1/\hat{G}$ (m/day)

Case	Equation	Transforming mechanism	Effective parameters	
			$\hat{g}$,	$\hat{K} = 1/\hat{g}$
6.2.1	1	$\hat{g}_1 = 0.6861g_1 + 0.3139g_2 + 0.0072g_3 - 0.0072g_4$	$\hat{g}_1 = 0.9989$,	$\hat{K}_1 = 1.0011$
	2	$\hat{g}_2 = -0.3451g_1 + 0.3451g_2 + 0.8157g_3 + 0.1843g_4$	$\hat{g}_2 = 5.9595$,	$\hat{K}_2 = 0.1678$
6.2.2	3	$\hat{g}_3 = 0.6861g_1 + 0.3139g_2 + 0.0072g_3 - 0.0072g_4$	$\hat{g}_3 = 8.4311$,	$\hat{K}_3 = 0.1186$
	4	$\hat{g}_4 = -0.3451g_1 + 0.3451g_2 + 0.8157g_3 + 0.1843g_4$	$\hat{g}_4 = -0.6351$,	$\hat{K}_4 = -1.5746$
6.2.5	5	$\hat{g}_5 = 0.5193g_1 + 0.3190g_2 + 0.1380g_3 + 0.0237g_4$	$\hat{g}_5 = 7.2516$,	$\hat{K}_5 = 0.1379$
6.2.6	6	$\hat{g}_6 = 0.6407g_1 + 0.3593g_2 + 0.0133g_3 - 0.0133g_4$	$\hat{g}_6 = 8.2034$,	$\hat{K}_6 = 0.1219$
	7	$\hat{g}_7 = -0.1891g_1 + 0.1891g_2 + 0.7802g_3 + 0.2198g_4$	$\hat{g}_7 = 0.1413$,	$\hat{K}_7 = 7.0757$
6.2.7	8	$\hat{g}_8 = 0.6076g_1 + 0.3924g_2 + 0.0091g_3 - 0.0091g_4$	$\hat{g}_8 = 8.0386$,	$\hat{K}_8 = 0.1244$
	9	$\hat{g}_9 = -0.0814g_1 + 0.0814g_2 + 0.8096g_3 + 0.1904g_4$	$\hat{g}_9 = 0.6830$,	$\hat{K}_9 = 1.4642$
6.2.8	10	$\hat{g}_{10} = 1 \times g_1 + 0.0948g_2 - 0.0743g_3 - 0.0205g_4$	$\hat{g}_{10} = 10.3734$,	$\hat{K}_{10} = 0.0964$
	11	$\hat{g}_{11} = 0 \times g_1 + 0.5612g_2 + 0.3673g_3 + 0.0715g_4$	$\hat{g}_{11} = 3.2862$,	$\hat{K}_{11} = 0.3043$

Contrary to seeing problem dependence as an obstacle or annoying factor, it is more profitable to consider it as a tool for investigation of geological objects. Different formulations of the model identification problems and corresponding transforming mechanisms carry information about the structures and properties of geological objects. They can even be applied during formulating and solving inverse problems. Geophysics is an example of such use of the phenomenon of problem dependence. The notion of apparent electrical resistivity corresponds to an effective parameter as defined in the hydrogeological model identification herein. Namely, the apparent specific electrical resistivity provides the exact difference of electrical potentials between the receiving electrodes for a given configuration of the current electrodes. Its value is calculated based on the assumption that the geological object is homogeneous with respect to the specific electrical resistivity. If the actual object is not homogeneous, changing the configuration of the current electrodes, which is equivalent to changing the boundary conditions (or locations of sources and sinks), leads to change of the apparent resistance. The pattern of this change can be used for qualitative or quantitative interpretation of the object structure.

Let us consider the following system of equations:

$$\begin{aligned} 0.6861g_1 + 0.3139g_2 + 0.0072g_3 - 0.0072g_4 &= 8.4311, \\ -0.3451g_1 + 0.3451g_2 + 0.8157g_3 + 0.1843g_4 &= -0.6351, \\ 0.6076g_1 + 0.3924g_2 + 0.0091g_3 - 0.0091g_4 &= 8.0386, \\ -0.0814g_1 + 0.0814g_2 + 0.8096g_3 + 0.1904g_4 &= 0.6930. \end{aligned} \tag{6.24}$$

System (6.24) is composed from Eqs. 3, 4, 8, 9 (Table 6.10). The actual hydraulic resistivities $g_{1\ldots4}$ are assumed to be unknown. Corresponding effective hydraulic resistivities, the right-hand terms, are found from observations and as such are known. Solving system (6.24) for the unknown actual resistivities and recalculating them for the actual hydraulic conductivities yields

$$K_1 = 0.1,\ K_2 = 0.2,\ K_3 = 0.9,\ K_4 = 1.0\ \text{m/day}. \tag{6.25}$$

These are the exact actual properties of the considered object.

Inverse problems are inherently incorrect. The source of incorrectness is errors in the coefficients making up the matrix of system (6.24) and in the right-hand vector. Solutions of systems such as system 6.3 depend strongly on the accuracy of the initial data and rounding errors (see Eq. 4.20). The above success is due to the fact that the made-up, artificial situation permits calculation of values of the affecting factors and effective parameters with accuracy of 14 digits. If solving the inverse problem with the data presented in Table 6.10, that is, with four significant digits, the result becomes

$$K_1 = 0.1,\ K_2 = 0.1997,\ K_3 = 0.9109,\ K_4 = 0.9622\ \text{m/day}, \tag{6.26}$$

which is still appropriate. If the system for finding the actual hydraulic resistivity is made up by Eqs. 3, 4, 6, and 7 from Table 6.10 and the pertinent values are rounded up to three digits after the decimal point, the obtained solution is not so good:

$$K_1 = 0.0997, \; K_2 = 0.2030, \; K_3 = 0.8137, \; K_4 = 1.4905 \text{ m/day}, \qquad (6.27)$$

though it may be acceptable, considering the usual accuracy of hydrogeological information. Some systems made up from other combinations of the four equations presented in Table 6.10 may yield much worse results.

In day-to-day practice, having four correct significant digits is an unavailable luxury. A more practical approach to solving our inverse problem is to use excessive systems of equations and solve them by the least-squares method; for example, the affecting factors in Eqs. 3–11 from Table 6.10 can be considered as independent variables and the unknowns the actual values g_1, g_2, g_3, and g_4 as coefficients of the linear regression

$$\hat{g}_j = g_1 w_{j1} + g_2 w_{j2} + g_3 w_{j3} + g_4 w_{j4}. \qquad (6.28)$$

(Due to the properties 1–3 of the affecting factors are not independent. This does not preclude considering them as such. However, the dependence of the affecting factors can simplify solution of inverse problems).

Applying the least-squares method to minimize the sum

$$s = \sum_{j=3}^{11} \left(g_1 w_{j1} + g_2 w_{j2} + g_3 w_{j3} + g_4 w_{j4} - \hat{g}_j \right)^2 \qquad (6.29)$$

yields a system of four equations for evaluating the regression coefficients g_1, g_2, g_3, and g_4. Solution of that system expressed in terms of the hydraulic conductivities is

$$K_1 = 0.0995, \; K_2 = 0.1981, \; K_3 = 0.8627, \; K_4 = 1.1594 \text{ m/day}. \qquad (6.30)$$

This approach to solving inverse problems, using the transforming mechanisms, is considered in more detail in Chap. 9.

Konikow and Bredehoeft (1992) claim that a site-specific validation "per se, is a futile objective." In my opinion, they are wrong if we stop looking at calibration as just the procedure for searching for the effective parameters of a given model to provide the best fit of the available observations and start seeing it as a procedure for systematic study of hydrogeological objects. The transforming mechanisms may become a tool for this kind of investigations, though I believe that other tools can be found also.

6.4 Borden Landfill

I think that Frind and Hokkanen (1987) assigned their recharge rate pattern and the steady-state water table for the part of the Borden site located down-gradient of the landfill ($x > 300$ m) in Sect. 4.4, taking into consideration the observed streamline

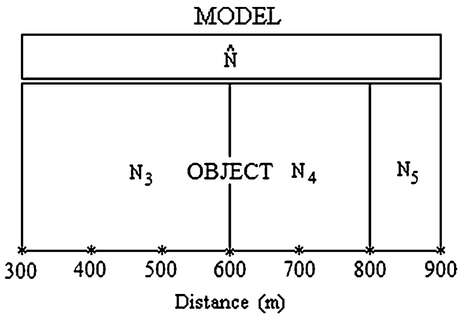

Fig. 6.7 Borden site: model homogeneous with respect to recharge rate

which coincides with the upper boundary of the contaminant plume. Then, they scaled the pattern to satisfy the known arrival time. The goal of this section is to obtain the mechanism transforming the rates N_3, N_4, and N_5 into one effective recharge rate $\hat{N}$ of the homogeneous simulation model for $x > 300$ m (Fig. 6.7).

The effective recharge rate $\hat{N}$ should provide the effective, as if steady-state, water table. [Note that, if the structure of the model of Frind and Hokkanen (1987) in Sect. 4.4 had been an exact replica of the Borden site, then effective recharge rates would be equal to the actual recharges, i.e., $\hat{N}_3 = N_3$, $\hat{N}_4 = N_4$ *and* $\hat{N}_5 = N_5$, and as shown in Sect. 5.3, the corresponding transforming mechanisms become trivial, with affecting factors $w_{1,1} = w_{2,2} = w_{3,3} = 1$, $w_{1,2} = w_{1,3} = w_{2,1} = w_{2,3} = w_{3,1} = w_{3,2} = 0$].

The transforming mechanisms for the homogeneous model can be presented as

$$\hat{N} = w_1 N_3 + w_2 N_4 + w_3 N_5, \tag{6.31}$$

where the affecting factors w_1, w_2, and w_3 sum to one. According to Eq. 4.35, the actual water table $H(x)$ for $x > x_{st}$ is described by the equation

$$H(x) = \frac{Q(x)}{Q_S}(H_S(x) - Y(x)) + Y(x), \tag{6.32}$$

where $H_S(x)$ is the streamline S elevation, $Y(x)$ is the aquifer base elevation, $Q(x)$ is the total flux, and $Q_S = Q(x_{st})$, where x_{st} is the coordinate of the point of streamline S on the water table.

The effective water table $\hat{H}(x)$ is described by the equation

$$\hat{H}(x) = \frac{\hat{Q}(x)}{Q_S}(H_S(x) - Y(x)) + Y(x), \tag{6.33}$$

where $\hat{Q}(x)$ is the effective total flux $x > x_{st}$. The effective value of the homogeneous recharge rate $\hat{N}$ minimize the sum

$$s = \sum_{i=1}^{n} \left(\hat{H}(x_i) - H(x_i)\right)^2, \tag{6.34}$$

Table 6.11 Data for evaluating the transforming mechanism for effective recharge rate

No.	x	H_S	Y	$u = H_S - Y$	$\hat{Q}$	Q
0	300	222.31	204.31	17.99	Q_S	Q_S
1	400	219.25	206.17	13.08	$Q_S + 100\hat{N}$	$Q_S + 100\,N_3$
2	500	218.26	209.55	8.71	$Q_S + 200\hat{N}$	$Q_S + 200\,N_3$
3	600	217.46	210.85	6.61	$Q_S + 300\hat{N}$	$Q_S + 300\,N_3$
4	700	216.07	211.33	4.74	$Q_S + 400\hat{N}$	$Q_S + 300\,N_3 + 100\,N_4$
5	800	215.47	211.86	3.61	$Q_S + 500\hat{N}$	$Q_S + 300\,N_3 + 200\,N_4$
6	900	215.67	212.79	2.88	$Q_S + 600\hat{N}$	$Q_S + 300\,N_3 + 200\,N_4 + 100\,N_5$

where x_i are the locations where the values $H(x)$, $Y(x)$, and $H_S(x)$ are observed. However, observations on $H(x)$ are not necessary and even may not exist in this case. Indeed, substituting Eqs. 6.32 and 6.33 into criterion (6.34) yields

$$s = \frac{1}{Q_S^2} \sum_{i=1}^{n} \left((\hat{Q}(x_i) - Q_i(x_i))(H_S(x_i) - Y(x_i)) \right)^2. \tag{6.35}$$

So, the problem is reduced to evaluating the effective recharge rate based on an observed streamline. According to the least-squares method, the effective recharge rate $\hat{N}$ is the solution of the equation

$$\sum_{i=1}^{n} \left((\hat{Q}(x_i) - Q(x_i))(H_S(x_i) - Y(x_i)) \right) \frac{\mathrm{d}\hat{Q}(\mathrm{x_i})}{\mathrm{d}\hat{N}} = 0. \tag{6.36}$$

Substituting the data from Table 6.11 into Eq. 6.36 and solving it for $\hat{N}$ yields Eq. 6.31 with $w_1 = 0.8005$, $w_2 = 0.1727$, and $w_3 = 0.0269$ summing to 1.0001. (The error of 0.0001 is due to rounding. Adding one more digit, i.e., putting $w_1 = 0.80045$, $w_2 = 0.17267$, $w_3 = 0.02688$, makes the sum equal to one.) So finally, the transforming mechanisms converting the recharge rates N_3, N_4, and N_5 into the effective recharge rate $\hat{N}$ is

$$\hat{N} = 0.8005N_3 + 0.1727N_4 + 0.0269N_5. \tag{6.37}$$

Substituting into Eq. 6.37 the recharge pattern $N_{1:5} = [5.85, 28.41, 10.20, 23.00, 8.36]$ cm/year (Table 4.4) satisfying the streamline shape and the travel times to $x = 900$ m and $x = 950$ m (about 39.1 and 40.2 years) yields the effective recharge

$$\hat{N} = 0.8005 \times 10.2 + 0.1727 \times 23 + 0.0269 \times 8.36 = 12.36\ \mathrm{cm/year}. \tag{6.38}$$

To obtain mechanism (6.37), we do not need the observation on the water table, and the total flux Q_S at $x = 300$ m. Taking into consideration the seasonal variability of the water table, which is expected to be greater than the variability of the streamline elevations, the water table obtained with the use of the effective recharge $\hat{N}$ seems to be a good first approximation. However, the above result

Table 6.12 Data for evaluating the transforming mechanism for effective recharge rate $\hat{N}$ ($rN = \hat{N}/Q_S$)

No.	x	H	$v = H - Y$	Y	H_S	$u = H_S - Y$	$\hat{Q}/Q_S$
0	300	222.31	17.99	204.31	222.31	17.99	1
1	400	222.23	16.06	206.17	219.25	13.08	$1 + 100\,rN$
2	500	222.11	12.56	209.55	218.26	8.71	$1 + 200\,rN$
3	600	221.95	11.09	210.85	217.46	6.61	$1 + 300\,rN$
4	700	221.72	10.39	211.33	216.07	4.74	$1 + 400\,rN$
5	800	221.42	9.56	211.86	215.47	3.61	$1 + 500\,rN$
6	900	221.04	8.24	212.79	215.67	2.88	$1 + 600\,rN$

$\hat{N} = 12.36\,\text{cm/year}$ can be checked by straightforward calculation of the effective recharge applying the observed water table. To this end it is necessary to minimize the criterion

$$s = \sum_{i=1}^{6} \left(\frac{\hat{Q}_i}{Q_S} (H_S(x_i) - Y(x_i)) - (H(H_S(x_i) - Y(x_i) - Y_i) \right)^2 \tag{6.39}$$

with $H(x)$ corresponding to the above-mentioned recharge pattern from Table 4.4 ($N_{1\ldots5}$ = 5.85, 28.41, 10.20, 23.00, and 8.36 cm/year). The data for calculation are presented in Table 6.12. Note also that the effective recharge rate of the model which is homogeneous with respect to recharge for $x > 300$ m must minimize the difference between the observed water table and the simulated one.

It follows from Eq. 6.39 that the minimum value of the criterion (6.39) depends on the ratio $\hat{Q}_i/Q_S$. Thus, the goal is to find the optimal value of this ratio, denoted here as rN. The standard least-squares technique leads to the equation

$$\begin{aligned} 100\left(u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2\right) rN &= u_1(v_1 - u_1) + 2u_2(v_2 - u_2) \\ &+ 3u_3(v_3 - u_3) + 4u_4(v_4 - u_4) + 5u_5(v_5 - u_5) + 6u_6(v_6 - u_6). \end{aligned} \tag{6.40}$$

According to Eq. 6.40, $rN = 0.0027$. Calculated based on recharge rates $N_{1\ldots2}$ = 5.85, 28.41 cm/year the total flux Q_S at $x = x_{\text{st}} = 300$ m is equal to 0.1253 m^2/day. Thus, the effective recharge rate is

$$\hat{N} = rN \times Q_s \times 100 \times 365 = 12.40\,\text{cm/year}. \tag{6.41}$$

The results obtained by Eqs. 6.38 and 6.41 are consistent, though based on slightly different data.

Thus, the transforming mechanism presented by Eq. 6.38, as expected, provides the effective parameter $\hat{N}$ for the discussed simulation model. The magnitude of the maximal error in reproducing the water table is less than 9.1 cm. However, the magnitude of the maximal error in evaluation the streamline starting at $x = 300$ m is too large, about 0.56 m (Fig. 6.8), since the streamline was not the goal of

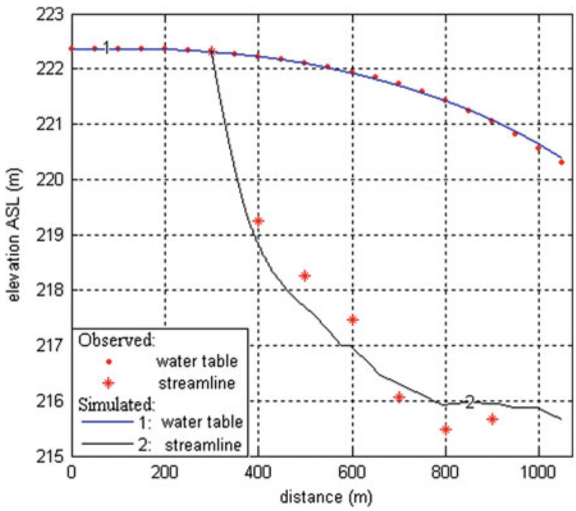

Fig. 6.8 Reproduction of observations by the homogeneous model

reproduction (providing one more illustration of the problem dependence of model identification). Nevertheless, the travel times to $x = 900$ and $x = 950$ m are equal to approximately 38.5 and 39.7 years, close to those found in Sect. 4.4 (39.1 and 40.2 years).

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Chapter 7
Examples of Nonlinear Transforming Mechanisms

Linear transforming mechanisms are rare in practical applications. Even the mechanisms presented in Sect. 6.2 were obtained by linearization of nonlinear mechanisms. Mathematical descriptions of the nonlinear mechanisms, and their inferences and applications are considerably more complicated. However, it is still possible to find simple examples for illustrations.

7.1 Simulation of Transient Filtration in a Two-Body Object by a Homogeneous Model: Problem Formulation

As shown in Sect. 4.3, a homogeneous model with constant hydraulic transmissivity cannot successfully represent the development of hydraulic heads for a long enough period in a confined aquifer consisting of two geological bodies with hydraulic transmissivities T_1 and T_2 (Fig. 7.1). However, the situation is different if we use an effective hydraulic transmissivity changing in time.

Let the aquifer have uniform distribution of hydraulic heads in the initial state: $h(x, 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L$ jumps to $h(2L, 0) = H_{2L.}$ At $x = 0$ the hydraulic head remains unchanged: $h(0, t) = H_0$. The instantaneous jump of the hydraulic head at $x = 2L$ initiates a process of change of the aquifer hydraulic heads. The goal is effective simulation of the hydraulic head at location $x = L$, using a homogeneous, one-block, model.

Filtration within two geological bodies, that is, within intervals [0, L] and [L, 2L], is described by two partial differential equations

$$\frac{\partial h(x,t)}{\partial t} = A_j \frac{\partial^2 h(x,t)}{\partial x^2} \quad j = 1, 2, \tag{7.1}$$

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_7,

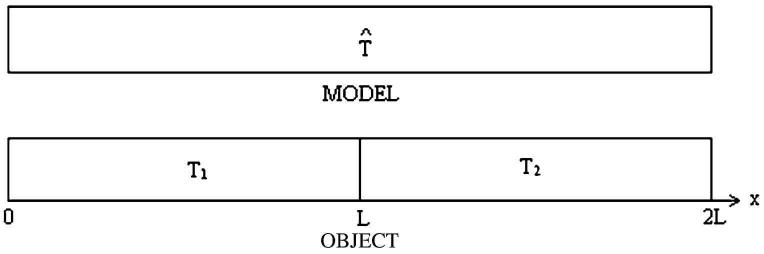


Fig. 7.1 Modeling a two-body object by a homogeneous model

where x and t are the distance and the time, $h(x, t)$ is the hydraulic head in intervals $[0, L]$ ($j = 1$) or $[L, 2L]$ ($j = 2$), $A_j = T_j/S$ is the hydraulic diffusivity of body j, T_j is its transmissivity, and S is the storativity, which for the sake of simplicity, is assigned equal to 0.1 for both bodies. The initial and boundary conditions are the following:

$$h(x, 0) = 0, \quad 0 \le x \le 2L, \tag{7.2}$$

$$h(0, t) = H_0 = 0, \quad \text{and} \quad h(2L, t) = H_{2L} = 1\,\text{m}. \tag{7.3}$$

(The values of the boundary conditions are assigned to make calculations simpler).

The inner boundary conditions on continuity of hydraulic head and flux exist at the boundary between the geological bodies at $x = L$

$$\begin{aligned} \lim(h(x,t))|_{x\to L} &= \lim(h(x,t))|_{L\leftarrow x} \\ T_1\left(\frac{\partial h(x,t)}{\partial x}\right)\Bigg|_{x\to L} &= T_2\left(\frac{\partial h(x,t)}{\partial x}\right)\Bigg|_{L\leftarrow x} \end{aligned} \tag{7.4}$$

The real world constructed in the above problem formulation is to be simulated by a homogeneous model. The simulation process is described by the equation

$$\frac{\partial \hat{h}(x,t)}{\partial t} = \hat{A}\frac{\partial^2 \hat{h}(x,t)}{\partial x^2}, \tag{7.5}$$

where $\hat{h}(x,t)$ is the effective hydraulic head at location x and at time instant t, $\hat{A} = \hat{T}/S$, and $\hat{T}$ is the effective hydraulic transmissivity. The model storativity S is assigned equal to 0.1.

The simulation must effectively reproduce the next hydraulic head, $\hat{h}(L, t_i) = \hat{h}_i$, based on the observed previous head $h(L, t_{i-1}) = h_{i-1}$. For simplicity, the time increment $\Delta t = t_i - t_{i-1}$ is kept constant. The simulations are to be conducted by explicit finite differences. The model must be effective in the time interval $[t_k, t_m]$ in the sense of least squares; that is, the simulated hydraulic heads must minimize the sum

$$s_{k,m} = \sum_{i=k}^{m}\left(\hat{h}_i - h_i\right)^2. \tag{7.6}$$

To this end, the effective hydraulic transmissivity, $\hat{T}_{k,m}$, the only parameter governing the simulation, must be found.

7.2 Explicit Numerical Simulation

There exists an analytical solution for the hydraulic heads in the above-formulated problem. However, to simplify obtaining the pertinent transforming mechanism, the explicit finite-difference method with the stencil presented in Fig. 7.2 is applied to simulate both the real-world and the homogeneous model. The equation for evaluating the real-world hydraulic head based on the immediately preceding observed hydraulic head is

$$h_i \approx h_{i-1} + \frac{\Delta t}{SL^2}((1 - h_{i-1})T_2 - h_{i-1}T_1). \tag{7.7}$$

The hydraulic heads simulated on the homogeneous aquifer model with effective hydraulic conductivity $\hat{T}_{k,m}$ can be obtained from Eq. 7.7 by putting $T_1 = T_2 = \hat{T}_{k,m}$,

$$\hat{h}_i \approx h_{i-1} + \frac{\Delta t}{SL^2}(1 - 2h_{i-1})\hat{T}_{k,m}. \tag{7.8}$$

Then, criterion (7.6) can be written as

$$s_{k,m} = \frac{\Delta t}{SL^2}\sum_{i=k}^{m}\left((1 - 2h_{i-1})\hat{T}_{k,m} - ((1 - h_{i-1})T_2 - h_{i-1}T_1)\right)^2. \tag{7.9}$$

Applying to criterion (7.9) the standard least-squares technique, that is, differentiating it with respect to $\hat{T}_{k,m}$ and equalizing the derivative to zero, yields

$$\hat{T}_{k,m} = -\frac{\sum_{i=k}^{m} h_{i-1}(1 - 2h_{i-1})}{\sum_{i=k}^{m}(1 - 2h_{i-1})^2}T_1 + \frac{\sum_{i=k}^{m}(1 - h_{i-1})(1 - 2h_{i-1})}{\sum_{i=k}^{m}(1 - 2h_{i-1})^2}T_2, \quad k > 0. \tag{7.10}$$

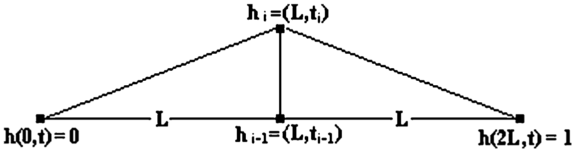
Equation 7.10 can be rewritten in terms of the affecting factors

$$\hat{T}_{k,m} = w_{1,[k,m]}T_1 + w_{2,[k,m]}T_2, \tag{7.11}$$

where the affecting factors $w_{1,[k,m]}$ and $w_{2,[k,m]}$ are

$$w_{1,[k,m]} = -\frac{\sum_{i=k}^{m} h_{i-1}(1 - 2h_{i-1})}{\sum_{i=k}^{m}(1 - 2h_{i-1})^2}, \quad w_{2,[k,m]} = \frac{\sum_{i=k}^{m}(1 - h_{i-1})(1 - 2h_{i-1})}{\sum_{i=k}^{m}(1 - 2h_{i-1})^2}, \quad k > 0. \tag{7.12}$$

Fig. 7.2 Four-point stencil for numerical modeling of the hydraulic heads



It is easy to check that the above affecting factors obey property 1 (Sect. 5.3, Eq. 5.5), summing to one. However, they can have different signs. If in interval $[t_k, t_m]$ all h_{i-1} are less than 0.5 m, then $w_{1,[k,m]}$ is negative and $w_{2,[k,m]}$ is positive. If in interval $[t_k, t_m]$ all h_{i-1} are greater than 0.5 m, then $w_{1,[k,m]}$ is positive and $w_{2,[k,m]}$ is negative. Therefore, the effective hydraulic transmissivities $\hat{T}_{k,m}$ are not statistics of the hydraulic conductivities T_1 and T_2, even though the affecting factors in Eq. 7.11 sum to one.

It is somehow more cumbersome to see the nonlinearity of mechanism (7.11), but in the case of the effective parameter $\hat{T}_{1,2}$ this is fairly obvious. It follows from the initial condition (7.2) and Eq. 7.7 that

$$h_0 = 0 \quad \text{and} \quad h_1 \approx \frac{\Delta t}{SL^2} T_2.$$

Substituting the above values in Eq. 7.12 yields

$$w_{1,[1,2]} = -\frac{\left(1 - 2\frac{\Delta t}{SL^2}T_2\right)\frac{\Delta t}{SL^2}T_2}{1 + \left(1 - 2\frac{\Delta t}{SL^2}T_2\right)^2}, \quad w_{2,[1,2]} = \frac{1 + \left(1 - \frac{\Delta t}{SL^2}T_2\right)\left(1 - 2\frac{\Delta t}{SL^2}T_2\right)}{1 + \left(1 - 2\frac{\Delta t}{SL^2}T_2\right)^2}.$$

Thus, the affecting factors $w_{1,[1,2]}$ and $w_{2,[1,2]}$ depend on T_2, demonstrating the nonlinearity of the corresponding transforming mechanism. Note that the mechanism does not depend on the transmissivity T_1. However, it could be demonstrated in the same way that T_1 appears in the transforming mechanisms $\hat{T}_{2,3}$, $\hat{T}_{1,3}$, and all others for which $m \geq 3$.

Let us simplify the problem even more, requesting that the effective transmissivity $\hat{T}_{i-1,i}$ should provide exact reproduction of the hydraulic head $h_i = h(L, t_i)$, at instant t_i based on the observed hydraulic head h_{i-1}, at instant t_{i-1}. Then the effective transmissivity $\hat{T}_{i-1,i}$ can be obtained straightforwardly from Eq. 7.10 or by equalizing the hydraulic heads presented by Eqs. 7.7 and 7.8:

$$\hat{T}_{i-1,i} = -\frac{h_{i-1}}{1 - 2h_{i-1}} T_1 + \frac{1 - h_{i-1}}{1 - 2h_{i-1}} T_2. \tag{7.13}$$

The affecting factors for the transforming mechanism presented by Eq. 7.13 are

$$w_{1,i} = -\frac{h_{i-1}}{1 - 2h_{i-1}}, \quad w_{2,i} = \frac{1 - h_{i-1}}{1 - 2h_{i-1}}. \tag{7.14}$$

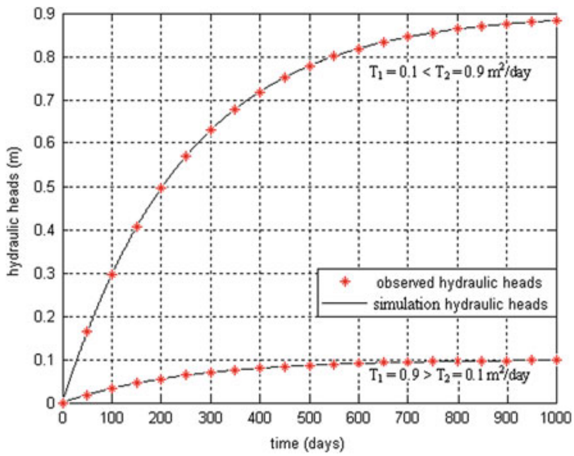


Fig. 7.3 Comparison of actual hydraulic heads obtained for a two-body object and homogeneous simulation model

It follows from expression (7.14) that the effective hydraulic conductivity $\hat{T}_{i-1,i}$ is not a statistic. Note that the affecting factors and the effective hydraulic transmissivity are not defined for the instant when the hydraulic head h_{i-1} is equal to 0.5 m. Note also that, at $t = 0$, the hydraulic head $h(0) = h_0 = 0$. Thus, the factor $w_{1,1} = 0$ and the effective hydraulic transmissivity $\hat{T}_{0,1} = T_2$.

The simulation results for two contrasting cases are presented in Fig. 7.3: one is the real world consisting of two bodies with hydraulic transmissivities $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day and the other with hydraulic transmissivities $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day. The main distinction between these cases is that in one of them the asymptotic value of the "observed" hydraulic heads h is equal to 0.1 m. It does not reach the crucial number $h = 0.5$ m. In the other the asymptote of the hydraulic heads is equal to 0.9 m, and the observed hydraulic heads exceed the crucial value $h = 0.5$ m.

Case 7.2.1 $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day. The homogeneous model works perfectly. The affecting factors $w_{1,i}$ and $w_{2,i}$ and the effective transmissivity $\hat{T}_{i-1,i}$ are presented in Fig. 7.4.

The upper left effective hydraulic transmissivity value is equal to $T_2 = 0.1$ m^2/day, which follows from Eq. 7.13.

The case demonstrates that the effective hydraulic transmissivities are incorrect geologically as well, approaching zero as time progresses.

Case 7.2.2 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day. The results are presented in Figs. 7.5 and 7.6. (The affecting factor $w_{1,i}$ is shown only, since $w_{2,i} = 1 - w_{1,i}$.) In this case there exists the instant $t_{0.5}$ such that $h(t_{0.5}) = 0.5$ m. At this instant the affecting factors and the effective hydraulic transmissivity do not exist. Thus, the effective transmissivity is deprived of both physical and geological meanings in

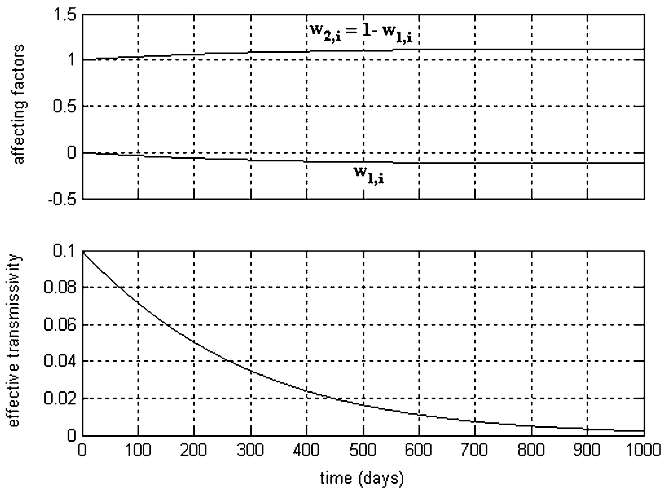


Fig. 7.4 Case 7.2.1: resulting affecting factors and effective hydraulic transmissivity

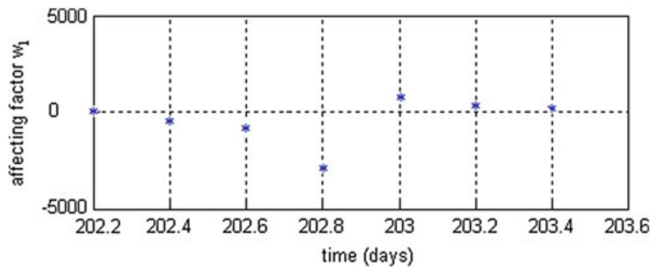


Fig. 7.5 Case 7.2.2: affecting factor $w_{1,i}$ in the vicinity of the crucial instant $t_{0.5}$

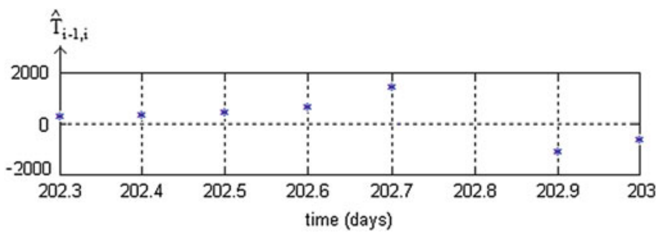


Fig. 7.6 Case 7.2.2: effective hydraulic transmissivity $\hat{T}_{i-1,i}$ in the vicinity of the crucial instant $t_{0.5}$

this case as well. However, this does not preclude its values from providing effective reproduction of real-world hydraulic heads.

As stated in Sect. 4.3, calibrating homogeneous models in a transient regime can permit simulation results fitting the observations satisfactorily for some short time interval. Use of effective hydraulic transmissivities changing in time permits obtaining considerably more accurate results. The two cases presented above clearly demonstrate that such effective parameters are not statistics, and even not geological or hydrogeological entities. They are just optimal characteristics of the corresponding systems and have no physical meaning.

7.3 Implicit Numerical Simulation

In the previous section an explicit finite-difference method was applied. To provide stability of the explicit numerical integration, the time increment Δt must be sufficiently small. An increment Δt of 0.1 days was selected in cases 7.2.1 and 7.2.2 for this reason. Although with the present status of automation, the duration of the time increment between measurements is not an issue, it may not be practical to use a very small value. However, the stable numerical solution for the problem formulated in Sect. 7.1 can be obtained for time increments of arbitrary duration by integrating Eq. 7.7 over time. Indeed, for infinitesimal ($\Delta t \to 0$), Eq. 7.7 can be rewritten, after separation of variables, as

$$\frac{\mathrm{d}h}{(1-h)T_2 - hT_1} = \frac{\mathrm{d}t}{SL^2}.$$

Integrating the above equation in intervals $[h_{i-1}, h_i]$ and $[t_{i-1}, t_i]$ yields

$$\int_{h_{i-1}}^{h_i} \frac{\mathrm{d}h}{T_2 - (T_1+T_2)h} = -\frac{1}{(T_1+T_2)} \ln(T_2 - (T_1+T_2)h)\Big|_{h_{i-1}}^{h_i} = \int_{t_{i-1}}^{t_i} \frac{\mathrm{d}t}{SL^2} = \frac{t_i - t_{i-1}}{SL^2}. \tag{7.15}$$

It follows from expression (7.15) (see Box 7.1) that

$$h_i = \frac{T_2}{T_1+T_2}\left\{1 - \left[1 - \left(\frac{T_1+T_2}{T_2}\right)h_{i-1}\right]\exp\left(-\frac{T_1+T_2}{SL^2}(t_i - t_{i-1})\right)\right\}. \tag{7.16}$$

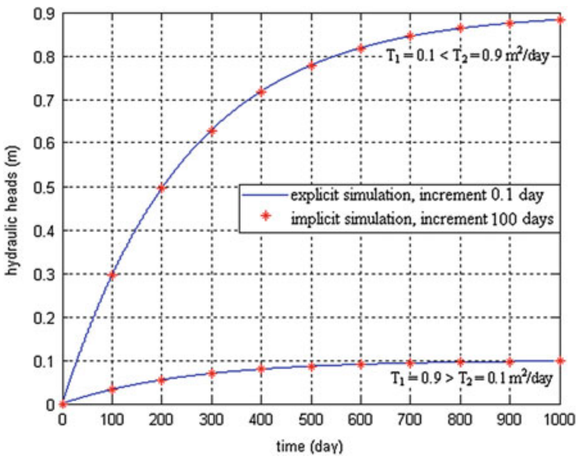


Fig. 7.7 Comparison of the explicit and implicit simulations

Text Box 7.1.
Inference of Eq. 7.16

Substituting in the right equality of expression (7.15) the limits of integration yields

$$\frac{1}{(T_1+T_2)}\ln(T_2-(T_1+T_2)h)\big|_{h_{i-1}}^{h_i} = -\frac{1}{(T_1+T_2)}\ln\frac{T_2-(T_1+T_2)h_i}{T_2-(T_1+T_2)h_{i-1}} = \frac{t_i-t_{i-1}}{SL^2}.$$

Potentiating the above equality gives

$$\frac{T_2-(T_1+T_2)h_i}{T_2-(T_1+T_2)h_{i-1}} = \exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right)$$

or

$$T_2-(T_1+T_2)h_i = (T_2-(T_1+T_2)h_{i-1})\exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right).$$

Solving this equation gives

$$h_i = \frac{T_2}{T_1+T_2} - \left(\frac{T_2}{T_1+T_2} - h_{i-1}\right)\exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right).$$

Factoring out the term T_2/T_1+T_2 yields Eq. 7.16

A comparison of the results obtained by Eqs. 7.7 and 7.16 is presented in Figs. 7.7 and 7.8 (the time increments for Eq. 7.16 are 100 days in Fig. 7.7 and 250 days in Fig. 7.8). In spite of the increase of the time increment by 1,000 and 2,500 fold, the results are identical.

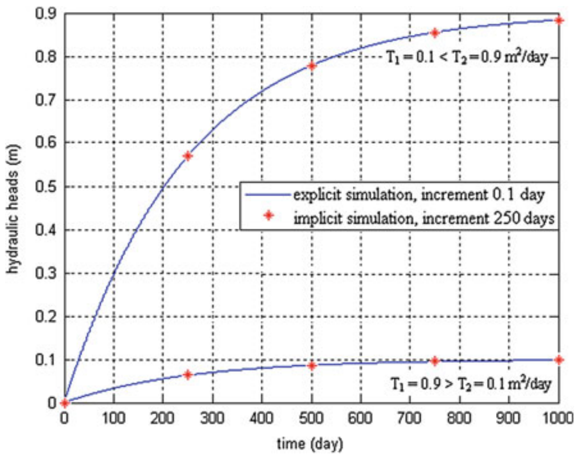


Fig. 7.8 Comparison of the explicit and implicit simulations

For a homogeneous simulation model $(T_1 = T_2 = \hat{T}_{i-1,i})$, Eq. 7.16 converts into

$$\hat{h}_i = \frac{1}{2}\left(1 - (1 - 2h_{i-1})\ \exp\left(-\frac{2\hat{T}_{i-1,i}}{SL^2}(t_i - t_{i-1})\right)\right). \tag{7.17}$$

The requirement for the model to be effective in the sense that $\hat{h}_i = h_i$ leads to the following choice for the effective hydraulic transmissivity:

$$\hat{T}_{i-1,i} = \frac{SL^2}{2(t_i - t_{i-1})}\ln\frac{1 - 2h_{i-1}}{1 - 2h_i}. \tag{7.18}$$

Substituting in Eq. 7.18 the hydraulic head h_i from Eq. 7.16 yields the following transforming mechanism:

$$\hat{T}_{i-1,i} = \frac{SL^2}{2(t_i - t_{i-1})}\ln\frac{1 - 2h_{i-1}}{1 - \frac{2}{T_1+T_2}\left\{T_2 - [T_2 - (T_1 + T_2)h_{i-1}]\exp\left(-\frac{T_1+T_2}{SL^2}(t_i - t_{i-1})\right)\right\}}. \tag{7.19}$$

The nonlinear transforming mechanism presented by Eq. 7.19 is difficult to analyze. However, it follows immediately from Eqs. 7.18–7.19 that the effective hydraulic transmissivity and the affecting factors are not defined for the case $T_1 < T_2$ at instant $t_{0.5}$ for which $h(t_{0.5}, L) = 0.5$ m. To the left and right of this instant, the effective hydraulic transmissivities and the affecting factors are continuous function of time and the hydraulic transmissivities T_1 and T_2. The hydraulic head $h(t_{0.5}, L) < 0.5$ always if $T_1 > T_2$. So, the effective transmissivity and the affecting factors are continuous in time in this case.

The affecting factors and the effective transmissivity for cases $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day and $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day with time increment of 50 days are presented in Figs. 7.9 and 7.10. As expected, in the first case ($T_1 = 0.9$ and $T_2 = 0.1$ m^2/day), the affecting factors and the effective transmissivity change

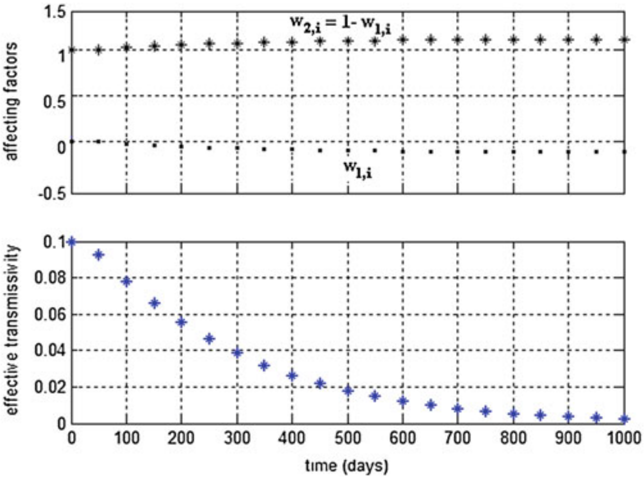


Fig. 7.9 Affected factors and effective hydraulic transmissivity $\hat{T}_{i-1,i}$: $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day

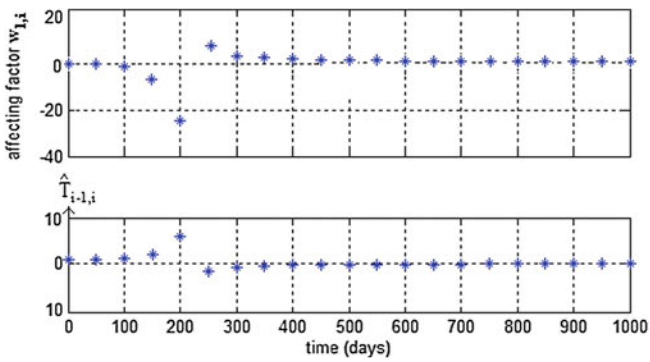


Fig. 7.10 Affected factor $w_{1,i}$ and effective hydraulic transmissivity $\hat{T}_{i-1,i}$: $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day

smoothly in time. The affecting factor $w_{1,i}$ takes nonpositive values. The factor $w_{2,i}$ always exceeds 1. The effective hydraulic transmissivity decreases smoothly from 0.1 to 0. In the case $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day, the affecting factors and the effective transmissivity are not defined in the vicinity of an instant at approximately 200 days (Figs. 7.10–7.12). Factually, there exist two different transforming mechanisms. One is valid for time interval [0, 200] and the other for interval ($\sim$200, 1,000] days. It should be noted also that the affecting factors and the effective transmissivities obtained implicitly vary less than those obtained explicitly.

Sections 7.2 and 7.3 demonstrate that values of the effective parameters and the transforming mechanisms depend on the methods of their evaluation. Although

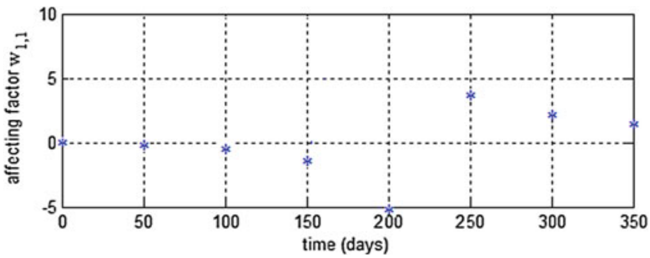


Fig. 7.11 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day: affected factor $w_{1,i}$

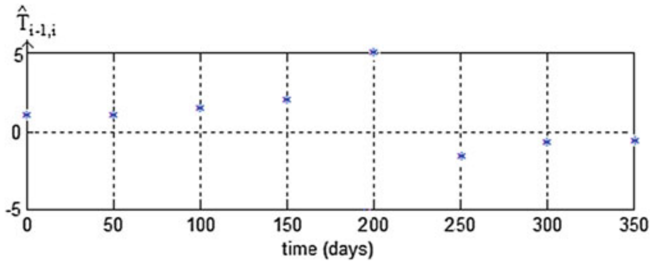


Fig. 7.12 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day: effective hydraulic transmissivity

some affecting factors of the mechanisms are negative, they sum to one. Thus, summing of the affecting factors to one does not warrant that the pertinent effective parameter is a statistic. The rightmost values of the effective hydraulic transmissivity have zero as an asymptote. This occurs because the hydraulic head approaches asymptotically its maximum value at $x = L$.

Most hydrogeologists hold that use of effective but incorrect values of geological parameters such as negative hydraulic conductivity or transmissivity in simulations is unacceptable. The question is what do we want: more accurate predictions and evaluations provided by physically incorrect parameters, or less accurate ones based on physically correct parameters? The physically correct parameters can be incorrect geologically, as demonstrated here, as well as in Chap. 6. Why is the use of geologically incorrect parameters acceptable? Just because we do not know that they are incorrect? Being an engineer, I prefer the accuracy and the tools that provide it. One must simply understand the systematic, optimizing, nature of effective model parameters. They are not physical entities and are effective only in the formulation in which they have been obtained. Any change in the simulation problem changes the system and requires reevaluation of the parameters. Applying effective parameters obtained for one simulation problem to a different one can cause misleading results, even when the differences between the problem formulations may not seem to be considerable.

Chapter 8
Evaluation of Transforming Mechanisms

In the examples of Chaps. 6 and 7 the transforming mechanisms were obtained analytically. Such a direct approach can be cumbersome and even not available in many situations. The two-level modeling introduced below is more universal and seems to be more practical.

8.1 Two-Level Modeling Concept

The following hypothetical situation is used to introduce the two-level modeling concept. Suppose that we are going to use a particular simulation model to predict the response of a particular geological object to a given impact. Information on the object is sparse, but we have complete information on many other geological sites with the same boundary conditions, impact, and monitoring network. Their responses to the impact have already been observed. Applying our simulation model to those sites, we could determine how different geological conditions affected the simulation results and use this knowledge; that is, we could see the sensitivity of our model to different geological conditions, which parts and properties of the geological objects (i.e., what information) are essential for effective prediction using our model, and how to assign its effective parameters. We could even abandon the model, if it is not satisfactorily effective, to try different ones.

In other words, we can accumulate specific engineering experience to deal with a specific problem. This does not eliminate the uncertainty of the simulation results, since the object of interest is not yet fully known. However, studies such as those would make our decisions related to prediction and its interpretation, including its uncertainty, more informed and focused. We acquire better understanding of what could go wrong and when, whether and when we have to update the simulation model, what additional feasible information could be necessary, etc.

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_8,

Unfortunately, we do not have objects with completely known geological surroundings, exactly the same impacts, monitoring networks, and long enough periods of observations. However, we can make them up as computer models. We can produce [using the terminology of McLaughlin and Wood (1988)] synthetic data, reference systems, and real worlds that are as complex as our computational resources permit, simulate their responses to a given impact, and compare those responses with the results yielded by a given simulation model. Simply speaking, we can make up some surrogate for the specific engineering experience.

There is nothing new about the use of artificial sites or synthetic data in groundwater modeling. In fact, the entire geostatistical approach with its made-up ensembles and other assumptions is based on them. McLaughlin and Wood (1988) use a synthetic, stochastically homogeneous ensemble of sites, or rather one site representing the mathematical expectation of the ensemble, to evaluate the accuracy of a proposed modeling study before extensive resources are committed to data collection and model development. Synthetic data are used by Zimmermann et al. (1998) and many others. Unfortunately, in practice, the relationship between artificial and actual sites is ambiguous, and the extension of the obtained results to real-world situations is difficult or even impossible (Eggleston et al. 1996).

The similarity of the reference systems to the geological object of interest is not necessary in the above hypothetical example. On the contrary, the diversity of conditions could be beneficial, permitting deeper understanding of the predictive problems. The reverse side of such diversity is the abundance of information, making it difficult to review and analyze. The transforming mechanisms are suggested as a generalization of the obtained information.

Thus, the idea behind the described approach, called here two-level modeling, is to investigate how the given predictive model performs when representing more complex geological models. In a sense, it corresponds to Monte Carlo simulations, only reversed. Routinely in Monte Carlo simulations “the object of the investigation is a model itself” (Gentle 1985). Varying the properties of a simulation model permits exploration of the sensitivity of the simulation results to the model’s parameters. However, the sensitivity of a model to its parameters tells us nothing about the model’s ability to represent the real geological objects. (Two exceptions are possible: low or high sensitivity of a model indicate that it may not be practical). In two-level modeling the structure of the geological model is fixed and the real worlds vary. This permits evaluation of how different factors, including the unknowns, can affect the simulation results.

The goal of two-level modeling is to evaluate the transforming mechanisms making the model parameter effective in the coupled predictive simulations, not just in calibration. The concept of two-level modeling can be described in general using the example of cases 6.2.1 and 6.2.2. The geological object, the real world, in these cases consists of four geological bodies and the geological model of two blocks. Pertinent transforming mechanisms for the first and second model blocks are described by the equations

Table 8.1 Set consisting of M subsets of observed effective and actual hydraulic resistivities

Effective parameters	Actual parameters
$\hat{g}_{1,1},\ \hat{g}_{1,2}$	$g_{1,1},\ g_{1,2},\ g_{1,3},\ g_{1,4}$
$\hat{g}_{2,1},\ \hat{g}_{2,2}$	$g_{2,1},\ g_{2,2},\ g_{2,3},\ g_{2,4}$
....	....
$\hat{g}_{m,1},\ \hat{g}_{m,2}$	$g_{m,1},\ g_{m,2},\ g_{m,3},\ g_{m,4}$
....	....
$\hat{g}_{M,1},\ \hat{g}_{M,2}$	$g_{M,1},\ g_{M,2},\ g_{M,3},\ g_{M,4}$

$$\begin{aligned}\hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4,\\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4,\end{aligned} \tag{8.1}$$

where $\hat{g}_1 = 1/\hat{K}_1 1$ and $\hat{g}_2 = 1/\hat{K}_2$ are the effective specific hydraulic resistivities of the first and second model blocks ($\hat{K}_1$ and $\hat{K}_2$ are the corresponding effective hydraulic conductivities), and $g_i = 1/K_i$ ($i = 1,\ldots, 4$) are the real-world specific hydraulic resistivities of the geological bodies (K_i are the corresponding hydraulic conductivities).

The transforming mechanisms described by Eqs. 8.1 are linear and independent of time. They can be interpreted as regressions, and their affecting factors $w_{j,i}$ ($j = 1, 2$ and $i = 1,\ldots, 4$) as coefficients of those linear regressions. To evaluate them, we need a large enough set consisting of subsets of data: $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ representing different real worlds and $\{\hat{g}_{m,1},\ \hat{g}_{m,2}\}$ representing the corresponding effective parameters of the predictive model. M such subsets are presented in Table 8.1. Independent variables $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ can be assigned arbitrarily, in particular to be generated as random values. Their knowledge permits the calculation of "observations" (Eqs. 6.7). The corresponding dependent variables $\{\hat{g}_{m,1},\ \hat{g}_{m,2}\}$ for a given set $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ can be calculated by solving system (6.10).

8.2 Examples of Evaluating Linear Transforming Mechanisms

Case 8.2.1 Let us come back to the problem described in Sect. 6.1: one-dimensional steady-state flow with constant recharge N to a fully penetrating trench at $X_0 = 0$ m in an unconfined aquifer on a horizontal aquitard (Fig. 8.1). The boundary conditions remain those assigned in Sect. 6.1.

As shown in Sect. 6.1, the effective resistivities for cases 6.2.1 and 6.2.2 are solutions of system (6.10), which in the case of uniform weighting ($p_1 = p_2 = p_3 = p_4 = 1$) takes the form

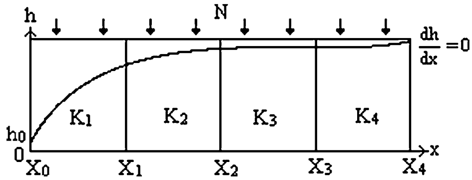


Fig. 8.1 One-dimensional steady-state flow to a fully penetrating trench in an unconfined aquifer

$$\begin{aligned}\hat{g}_1 &= 0.5635\left(h_1^2-h_0^2\right)+0.9659\left(h_2^2-h_0^2\right)+0.1546\left(h_3^2-h_0^2\right)-0.1159\left(h_4^2-h_0^2\right),\\ \hat{g}_2 &= -1.8931\left(h_1^2-h_0^2\right)-3.2454\left(h_2^2-h_0^2\right)+1.4005\left(h_3^2-h_0^2\right)+2.9491\left(h_4^2-h_0^2\right).\end{aligned} \tag{8.2}$$

Equations 8.2 permit evaluation of the effective values $\hat{g}_1$ and $\hat{g}_2$ for any subset m of the real-world hydraulic resistivities $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$, if corresponding squared thicknesses of the aquifer are known (calculated by Eqs. 6.7).

M such subsets are presented in Table 8.1. Equations 8.1 can be rewritten for convenience as one equation

$$\hat{g}_{m,j} = w_{j,1}g_{m,1} + w_{j,2}g_{m,2} + w_{j,3}g_{m,3} + w_{j,4}g_{m,4}, \quad j = 1, 2, \tag{8.3}$$

where the index j defines the model block and $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$ are the randomly assigned hydraulic resistivities. Since the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$ of the linear transforming mechanisms do not depend on the real-world hydraulic resistivities, they can be interpreted as regression coefficients of the regression represented by Eq. 8.3, and evaluated by the standard least-squares technique, that is, by minimizing the sum

$$s_j = \sum_{m=1}^{M} \left(w_{j,1}g_{m,1} + w_{j,2}g_{m,2} + w_{j,3}g_{m,3} + w_{j,4}g_{m,4} - \hat{g}_{m,j}\right)^2, \tag{8.4}$$

where M is the number of sets $\{g_{m,1\ldots4}\}$ assigned randomly. The least-squares technique leads to two systems (j = 1, 2) of linear equations for finding coefficients $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$:

$$\begin{aligned}
&w_{j,1}\sum_{m=1}^{M} g_{m,1}^2 + w_{j,2}\sum_{m=1}^{M} g_{m,1}g_{m,2} + w_{j,3}\sum_{m=1}^{M} g_{m,1}g_{m,3} + w_{j,4}\sum_{m=1}^{M} g_{m,1}g_{m,4} = \sum_{m=1}^{M} g_{m,1}\hat{g}_{m,j},\\
&w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,2} + w_{j,2}\sum_{i=1}^{M} g_{m,2}^2 + w_{j,3}\sum_{i=1}^{M} g_{m,2}g_{m,3} + w_{j,4}\sum_{i=1}^{M} g_{m,2}g_{m,4} = \sum_{i=1}^{M} g_{m,2}\hat{g}_{m,j},\\
&w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,3} + w_{j,2}\sum_{i=1}^{M} g_{m,2}g_{m,3} + w_{j,3}\sum_{i=1}^{M} g_{m,3}^2 + w_{j,4}\sum_{i=1}^{M} g_{m,3}g_{m,4} = \sum_{i=1}^{M} g_{m,3}\hat{g}_{m,j},\\
&w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,4} + w_{j,2}\sum_{i=1}^{M} g_{m,2}g_{m,4} + w_{j,3}\sum_{i=1}^{M} g_{m,3}g_{m,4} + w_{j,4}\sum_{i=1}^{M} g_{m,4}^2 = \sum_{i=1}^{M} g_{m,4}\hat{g}_{m,j}.
\end{aligned} \tag{8.5}$$

Solving system (8.5) yields the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$.

The resulting transforming mechanisms obtained with $M = 50$, 100, and 1,000 are exactly those obtained analytically for cases 6.2.1 and 6.2.2:

$$\begin{aligned} \hat{g}_1 &= \quad 0.6861 g_1 + 0.3139 g_2 + 0.0072 g_3 - 0.0072 g_4, \\ \hat{g}_2 &= -0.3451 g_1 + 0.3451 g_2 + 0.8155 g_3 + 0.1845 g_4. \end{aligned} \tag{8.6}$$

Case 8.2.2 Let us consider the above example only with a more complex piecewise-homogeneous real world. It comprises eight geological bodies with boundaries at locations $X_0 = 0$, $X_1 = 12.5$, $X_2 = 25$, $X_3 = 37.5$, $X_4 = 50$, $X_5 = 62.5$, $X_6 = 75$, $X_7 = 87.5$, and $X_8 = 100$ m. The hydraulic conductivities K_i are constant within intervals $[X_{i-1}, X_i]$: K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8. The two-block geological model has a boundary between the homogeneous blocks at $X_4 = 50$.

The monitoring network is located at the same four locations: $X_2 = 25$, $X_4 = 50$, $X_6 = 75$, and $X_8 = 100$ m. The criterion of efficiency remains the same (Eq. 6.6). Under the assumption of uniform weighting of observations, it can be rewritten as

$$s = \sum_{i=1}^{4} \left(\hat{h}_{2i}^2 - h_{2i}^2\right)^2. \tag{8.7}$$

Equation 6.4 for calculation of the real-world observed squared water table elevations at the boundaries of geological bodies takes the form

$$h_i^2 = h_{i-1}^2 + \frac{N}{K_i}(2X_8 - X_i - X_{i-1})(X_i - X_{i-1}). \tag{8.8}$$

The following equations describe the "observations" at locations X_i ($i = 1$–8) for $N = 0.0001$ m/day ($g_i = 1/K_i$):

$$\begin{aligned} h_1^2 &= h_0^2 + 0.2344\,g_1 \\ h_2^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 \\ h_3^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 \\ h_4^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 + 0.1406\,g_4 \\ h_5^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 + 0.1406\,g_4 + 0.1094\,g_5 \\ h_6^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 + 0.1406\,g_4 + 0.1094\,g_5 \\ &\quad + 0.0781\,g_6 \\ h_7^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 + 0.1406\,g_4 + 0.1094\,g_5 \\ &\quad + 0.0781\,g_6 + 0.0469\,g_7 \\ h_8^2 &= h_0^2 + 0.2344\,g_1 + 0.2031\,g_2 + 0.1719\,g_3 + 0.1406\,g_4 + 0.1094\,g_5 \\ &\quad + 0.0781\,g_6 + 0.0469\,g_7 + 0.0156\,g_8 \end{aligned} \tag{8.9}$$

Since the simulation model, the observation network, and the criterion of goodness of fit stay the same, finding the effective hydraulic resistivities (Eq. 8.2) need only change in enumeration of the observations:

$$\begin{aligned}\hat{g}_1 &= 0.5635\left(h_2^2 - h_0^2\right) + 0.9659\left(h_4^2 - h_0^2\right) + 0.1546\left(h_6^2 - h_0^2\right) - 0.1159\left(h_8^2 - h_0^2\right),\\ \hat{g}_2 &= -1.8931\left(h_2^2 - h_0^2\right) - 3.2454\left(h_4^2 - h_0^2\right) + 1.4005\left(h_6^2 - h_0^2\right) + 2.9491\left(h_8^2 - h_0^2\right).\end{aligned} \tag{8.10}$$

The regression equations relating the real-world hydraulic resistivities and the effective hydraulic conductivities of two model blocks differ from Eqs. 8.1 by the numbers of independent variables g_i and regressions coefficients $w_{1,i}$ and $w_{2,i}$ representing the affecting factors:

$$\begin{aligned}\hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4 + w_{1,5}g_5 + w_{1,6}g_6 + w_{1,7}g_7 + w_{1,8}g_8,\\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4 + w_{2,5}g_5 + w_{2,6}g_6 + w_{2,7}g_7 + w_{2,8}g_8.\end{aligned} \tag{8.11}$$

The standard least-squares technique applied for evaluating the affecting factors leads to two linear systems, each consisting of an equation with eight regression coefficients. Generating randomly the real-world data $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$, $g_{m,5}$, $g_{m,6}$, $g_{m,7}$, $g_{m,8}$ permits the calculation of the squared water table elevations $h^2_{m,2}$, $h^2_{m,4}$, $h^2_{m,6}$, and $h^2_{m,8}$, the effective hydraulic conductivities $\hat{g}_{m,j}$, and finally the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$, $w_{j,5}$, $w_{j,6}$, $w_{j,7}$, $w_{j,8}$. For the situation corresponding to cases 6.2.1 and 6.2.2 and the "real world" consisting of eight geological bodies, the results are the transforming mechanisms

$$\begin{aligned}\hat{g}_1 &= 0.3676g_1 + 0.3185g_2 + 0.1727g_3 + 0.1413g_4 + 0.0042g_5 + 0.0030g_6 - 0.0054g_7 - 0.0018g_8,\\ \hat{g}_2 &= -0.1849g_1 - 0.1602g_2 + 0.1899g_3 + 0.1553g_4 + 0.4759g_5 + 0.3397g_6 + 0.1383g_7 + 0.0461g_8.\end{aligned} \tag{8.12}$$

The mechanisms described by Eqs. 8.12 have the properties of the transforming mechanisms described by Eqs. 5.5–5.6. Indeed, the affecting factors belonging to the evaluated blocks $w_{1,1}$, $w_{1,2}$, $w_{1,3}$, $w_{1,4}$ and $w_{2,5}$, $w_{2,6}$, $w_{2,7}$, $w_{2,8}$ sum to one, and the affecting factors belonging to the affecting blocks $w_{1,5}$, $w_{1,6}$, $w_{1,7}$, $w_{1,8}$ and $w_{2,1}$, $w_{2,2}$, $w_{2,3}$, $w_{2,4}$ sum to zero. Besides, the affecting factors are additive. Thus, if $K_1 = K_2$, $K_3 = K_4$, $K_5 = K_6$, $K_7 = K_8$, Eqs. 8.12 convert into Eqs. 8.6.

Note that properties 1 and 2 of the transforming mechanisms (Sect. 5.3) permit simplification of the evaluation of the affecting factors, decreasing their numbers. For example, regressions (8.1) can be rewritten as

$$\begin{aligned}w_{1,1}(g_1 - g_2) + w_{1,3}(g_3 - g_4) &= \hat{g}_1 - g_2,\\ w_{2,1}(g_1 - g_2) + w_{2,3}(g_3 - g_4) &= \hat{g}_2 - g_4.\end{aligned} \tag{8.13}$$

Applying the least-squares method to the first Eq. 8.13 leads to a system of two equations for evaluating $w_{1,1}$ $(w_{1,2} = 1 - w_{1,1})$ and $w_{1,3}$ $(w_{1,4} = -w_{1,3})$.

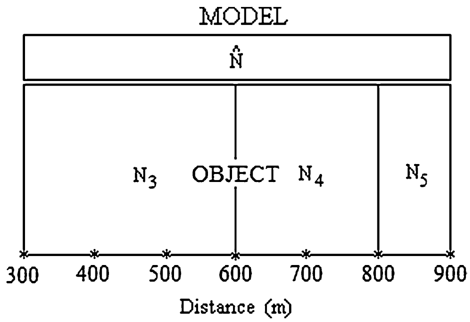


Fig. 8.2 Borden site and its homogeneous model with respect to the recharge rate

The second equation yields a system of two equations for evaluating $w_{2,1}$ ($w_{2,2} = -\, w_{2,1}$) and $w_{2,3}$ ($w_{2,4} = 1 - w_{2,3}$).

8.3 Transforming Mechanisms for Effective Recharge Rates at Borden Landfill

Let us come back to the problem described in Sect. 6.4, where the mechanism for converting three recharge rates in the effective recharge of a homogeneous model simulating the water table within the Borden site was obtained analytically. To this end, the available observations on the streamline starting at $x = 300$ m and the aquifer base elevations are used. The effective recharge rate $\hat{N}$ was calculated, using additionally the water table elevation, providing satisfactory reproduction of the streamline and the arrival time. Here, the transforming mechanism is evaluated by two-level modeling. The technique applied is exactly as described in the previous section.

This time the goal is to obtain the affecting factors (w_1, w_2, and w_3) of the transforming mechanism

$$\hat{N} = w_1 N_3 + w_2 N_4 + w_3 N_5, \tag{8.14}$$

where $\hat{N}$ is the effective recharge rate of the homogeneous model and N_3, N_4, and N_5 are the actual recharge rates (Fig. 8.2). For subset m of the independent variables N_3, N_4, N_5, relationship (8.14) takes the form

$$\hat{N}_m = w_1 N_{m,3} + w_2 N_{m,4} + w_3 N_{m,5}. \tag{8.15}$$

This can be interpreted as a linear regression in which the affecting factors w_1, w_2, w_3 can be evaluated as regression coefficients. Thus, first, M sets of recharge patterns $\{N_{3:5}\}$ and corresponding to them M sets of effective recharge rates$\{\hat{N}\}$ should be accumulated. (M must be a large enough number). Then a redundant system of equations such as Eq. 8.15 can be made up and solved for the affecting factors w_1, w_2, w_3 by the least-squares method.

Table 8.2 Data for evaluating effective recharge rate $\hat{N}_m$

No.	x	H_S	Y	$u = H_S - Y$	Q_m	$\hat{Q}_m$
0	300	222.31	204.31	204.31	Q_S	Q_S
1	400	219.25	206.17	206.17	$Q_S + 100N_{m,3}$	$Q_S + 100\hat{N}_m$
2	500	218.26	209.55	209.55	$Q_S + 200N_{m,3}$	$Q_S + 200\hat{N}_m$
3	600	217.46	210.85	210.85	$Q_S + 300N_{m,3}$	$Q_S + 300\hat{N}_m$
4	700	216.07	211.33	211.33	$Q_S + 300N_{m,3} + 100N_{m,4}$	$Q_S + 400\hat{N}_m$
5	800	215.47	211.86	211.86	$Q_S + 300N_{m,3} + 200N_{m,4}$	$Q_S + 500\hat{N}_m$
6	900	215.67	212.79	212.79	$Q_S + 300N_{m,3} + 200N_{m,4} + 100N_{\mathrm{m},5}$	$Q_S + 600\hat{N}_m$

Subsets $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ can be generated randomly. The problem is to evaluate the recharge rate$\hat{N}_m$ providing effective reproduction of the water table. The effective recharge rates should be obtained based on the generated recharge rate $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ and data presented in Table 8.2. Since the randomly picked recharge rates $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ are known, there is no need to resort to an as-if steady-state water table and its effective simulation (Eqs. 6.32–6.33). So, the effective recharge patterns $\hat{N}_m$ can be evaluated by minimization of criterion (6.36), which for working with subsets $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ and $\hat{N}_m$ can be rewritten as

$$s_m = \sum_{i=1}^{6} \left(\left(\hat{Q}_{m,i} - Q_{m,i} \right) \left(H_{S,i} - Y_i \right) \right)^2. \tag{8.16}$$

The standard least-squares technique leads to the equation

$$\begin{aligned} &\left(u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2\right)\hat{N}_m \\ &\quad = \left(u_1^2 + 4u_2^2 + 9u_3^2 + 12u_4^2 + 15u_5^2 + 18u_6^2\right)N_{m,3} \\ &\qquad + \left(4u_4^2 + 10u_5^2 + 12u_6^2\right)N_{m,4} + 6u_6^2 N_{m,5}. \end{aligned} \tag{8.17}$$

So

$$\hat{N}_m = \frac{\begin{aligned}&\left(u_1^2 + 4u_2^2 + 9u_3^2 + 12u_4^2 + 15u_5^2 + 18u_6^2\right)N_{m,3} \\ &\quad + \left(4u_4^2 + 10u_5^2 + 12u_6^2\right)N_{m,4} + 6u_6^2 N_{m,5}\end{aligned}}{u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2}. \tag{8.18}$$

The coefficients in terms containing $N_{m,3\ldots5}$ are made up from observations. They do not depend on the recharge they are equal to those presented in Eq. 6.37, though the corresponding effective recharges $\hat{N}_m$ are different. However, such convenience is not always available, and it may be easier to apply the two-level modeling exactly as done in the previous section. The affecting factors w_1, w_2, w_3 are those minimizing the sum

$$s = \sum_{m=1}^{M} \left(\hat{N}_m - w_1 N_{m,3} - w_2 N_{m,4} - w_3 N_{m,5}\right)^2. \quad (8.19)$$

The standard least-squares technique leads to the following system of linear equations for evaluating the affecting factors:

$$\begin{aligned}
w_1 \sum_{m=1}^{M} N_{m,3}^2 + w_2 \sum_{m=1}^{M} N_{m,3} N_{m,4} + w_3 \sum_{m=1}^{M} N_{m,3} N_{m,5} &= \sum_{m=1}^{M} N_{m,3} \hat{N}_m, \\
w_1 \sum_{m=1}^{M} N_{m,4} N_{m,3} + w_2 \sum_{m=1}^{M} N_{m,4}^2 + w_3 \sum_{m=1}^{M} N_{m,4} N_{m,5} &= \sum_{m=1}^{M} N_{m,4} \hat{N}_m, \\
w_1 \sum_{m=1}^{M} N_{m,5} N_{m,3} + w_2 \sum_{m=1}^{M} N_{m,5} N_{m,4} + w_3 \sum_{m=1}^{M} N_{m,5}^2 &= \sum_{m=1}^{M} N_{m,5} \hat{N}_m.
\end{aligned} \quad (8.20)$$

Solving system (8.20) yields the affecting factors $\{w_1, w_2, w_3\}$, which for M equal 10, 100, and 1,000 stay the same:

$$\{w_1 = 0.8005, w_2 = 0.1727, w_3 = 0.0269\}.$$

That is, the affecting factors are exactly those obtained in Sect. 6.4 (Eq. 6.37).

The explicit use of the properties of the transforming mechanism can simplify evaluation of the affecting factors, as shown in the previous section. In particular, since the affecting factors sum to one, one of them can be expressed through two others. So, instead of system (8.20) consisting of three equations, it is possible to work with a system consisting of two equations.

It may seem that, in the case of linear transforming mechanisms, two-level modeling is more complicated than their analytical deduction in Chap. 6. However, when geological objects and the corresponding simulation model become more complex, the situation may change. Besides, two-level modeling may work when there are no observed data yet, i.e., before starting field research, as shown in Sect. 8.2, or with data whose accuracy is low, as with the data on the water table in the Borden site. The procedures of the two-level modeling reveal more information on objects. They are easier to be standardized and programmed.

8.4 Two-Level Modeling for Nonlinear Transforming Mechanisms

Problems involving nonlinear transforming mechanisms are considerably more complex than those involving linear mechanisms, since nonlinear mechanisms depend on the actual distributions of the actual properties (geological bodies). There is no developed methodology for their evaluation at this moment. However, some notions on how this could be done are demonstrated below based on the conceptual examples of Sect. 7.3.

Let a two-body geological object be simulated by a one-block model. To simulate effectively the hydraulic heads $h(t, L)$ under the boundary conditions $h(t, 0) = 0$ and $h(t, 2L) = 1$, we have to use an effective hydraulic transmissivity varying in time. As shown in Sect. 7.3, the pertinent effective hydraulic conductivities are described by Eq. 7.18, which is repeated here:

$$\hat{T}_{i-1,i} = \frac{SL^2}{2\Delta t}\ln\frac{1-2h_{i-1}}{1-2h_i} \tag{8.21}$$

[$S = 0.1$ is the storativity, $h(t_{i-1}, L)$ and $h(t_i, L)$ are the observed hydraulic heads at $L = 50$ m and instants t_{i-1} and t_i.] Equation 8.21 permits evaluation of the effective transmissivity $\hat{T}_{i-1,i}$, which reproduces exactly the hydraulic head $h(t_i, L)$ based on the known hydraulic head $h(t_{i-1}, L)$. This result applies for the implicit formulation of the simulation problem and is valid for an arbitrary time increment Δt between observations. In the example discussed below, $\Delta t = t_{\mathrm{i}} - t_{i-1}$ is equal to 7 days.

Equation 8.21 assumes that both hydraulic heads $h(t_{i-1}, L)$ and $h(t_i, L)$ are known; that is, Eq. 8.21 is a tool for calibration. As we know, the effective transmissivities depend on time. So, the goal should be to extrapolate them beyond the period of calibration. This is possible since, as follows from Eq. 8.21, the effective transmissivity is a continuous function of $h(t_{i-1}, L)$ and $h(t_i, L)$, and consequently of time, besides the instant when $h(t_{i-1}, L) = 0.5$, in our case. For this reason, we can expect that the effective transmissivity evaluated by Eq. 8.21 remains close to efficiency for some time beyond the calibration period. As soon as monitoring reveals that the simulation results become unsatisfactory, the simulation model must be recalibrated.

Case 8.4.1 The hydraulic transmissivity of the first body is greater than that of the second one. (To make the "observations," the transmissivities T_1 and T_2 are assigned equal to 0.9 and 0.1 m^2/day, respectively, in this case). The model has been calibrated on the 13 available hydraulic heads obtained during the first 13 weeks (91 days) of observation. The results are presented in Fig. 8.3.

The calibration is an obvious success. To extrapolate its results beyond the period of calibration we need to describe the time dependence of the effective transmissivity explicitly. This can be done in many ways. The approximation (regression) presented in Fig. 8.3 is a polynomial of third degree

$$\begin{aligned}\hat{T} \approx & -1.0833\times10^{-10}(t-\bar{t})^3 + 3.7356\times10^{-7}(t-\bar{t})^2 - 2.8554 \\ & \times 10^{-4}(t-\bar{t}) + 0.0862,\end{aligned} \tag{8.22}$$

where $\bar{t} = 49$ days.

During about 60 weeks (420 days) the model worked more than satisfactorily (Fig. 8.4). Then, a systematic deviation appears between the simulation results and the observations. If the deviations are not permissible, the model must be recalibrated based on all available data. Let the new approximation be a polynomial of

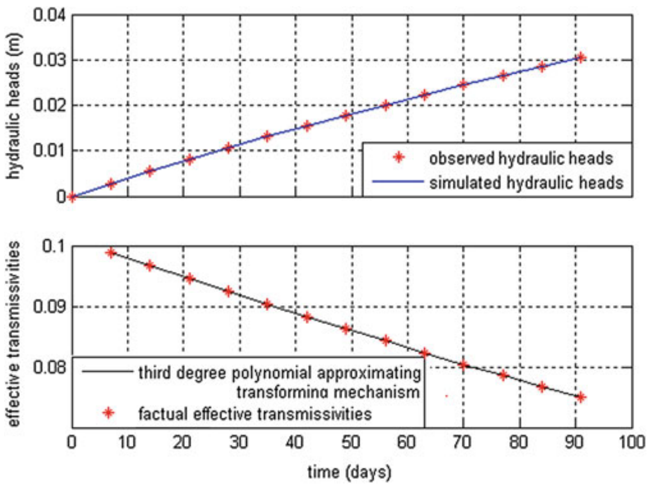


Fig. 8.3 Case 8.4.1: calibration on data related to the first 13 weeks. The effective hydraulic transmissivity given in m^2/day

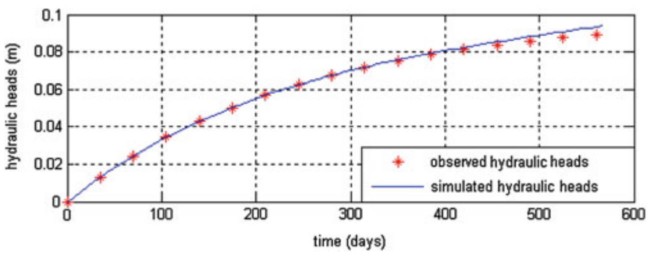


Fig. 8.4 Case 8.4.1: extrapolating simulations beyond period of calibration to the 81th week, applying the transforming mechanisms described by Eq. 8.22

fourth order. The least-squares method applied to the 81 weeks of "observations" yields

$$\hat{T} \approx -3 \times 10^{-14}(t-\bar{t})^4 - 2.0173 \times 10^{-10}(t-\bar{t})^3 + 2.3536 \times 10^{-7}(t-\bar{t})^2 - 1.3809 \times 10^{-4}(t-\bar{t}) + 0.0372, \quad (8.23)$$

where $\bar{t} = 287$ days.

The results of recalibration and extrapolation of the transforming mechanisms described by Eq. 8.23 on the entire prediction period, 1,000 days, are presented in Figs. 8.5 and 8.6. They reveal that there is no need for additional model recalibration.

By the way, location $x = 50$ m, convenient for illustration, is not the best for monitoring in this case. The hydraulic heads $h(t, L)$ approach the value 0.1 asymptotically. The closer the observed hydraulic heads are to this value, the less informative they become. To the right from that location, say, at $x = 75$ m, the process of development of the hydraulic heads is more dynamic and informative.

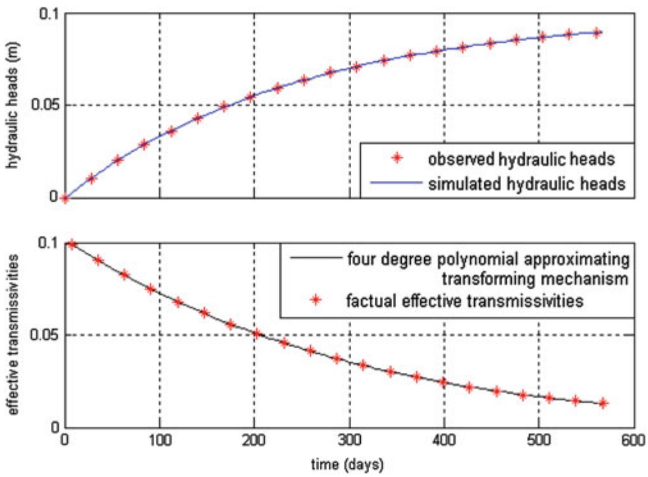


Fig. 8.5 Case 8.4.1: recalibration on data related to the first 81 weeks. The effective hydraulic transmissivity given in m^2/day

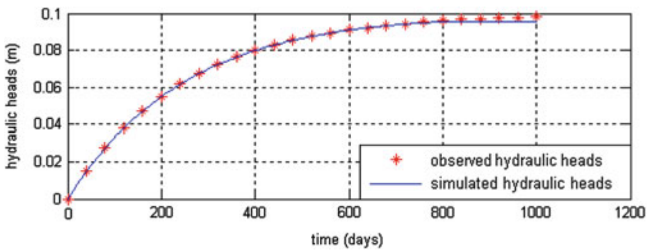


Fig. 8.6 Case 8.4.1: extrapolating simulations beyond period of calibration (81 weeks), applying the transforming mechanisms described by Eq. 8.23

Case 8.4.2 The hydraulic transmissivity of the first body is less than that of the second body. To make the "observations," $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day are assigned in this case. This case differs from the previous one. Developing in time, the hydraulic heads exceed the critical value $h(t, L) = 0.5$. According to Eq. 8.21 the effective hydraulic transmissivity as a function of time is discontinuous at that instant. Thus, two different transforming mechanisms have to be applied for simulation: one for the period when $h(t, L)$ is less than 0.5 and the other for the period when $h(t, L)$ exceeds 0.5.

The model has been calibrated on the 13 available hydraulic heads obtained during the first 13 weeks of observations. The results of calibration and the corresponding transforming mechanism are presented in Fig. 8.7. They seem to be quite satisfactory. To extrapolate those results from the development of the hydraulic heads beyond the period of calibration we need to describe the time

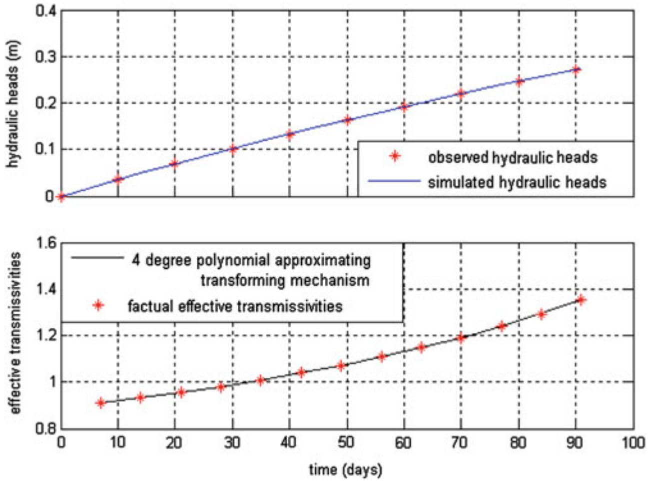


Fig. 8.7 Case 8.4.2: calibration on data related to the first 13 weeks

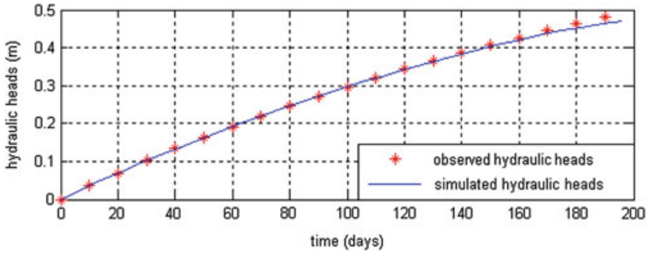


Fig. 8.8 Case 8.4.2: extrapolating simulations beyond period of calibration to the 28th week, applying the transforming mechanisms described by Eq. 8.24

dependence of the effective transmissivity mathematically. It seems that the regression presented in Fig. 8.7

$$\hat{T} \approx 1.4589 \times 10^{-9}(t-\bar{t})^4 + 2.2495 \times 10^{-7}(t-\bar{t})^3 + 3.2093 \times 10^{-5}(t-\bar{t})^2 + 4.8893 \times 10^{-3}(t-\bar{t}) + 1.0714, \quad (8.24)$$

where $\bar{t} = 49$ days, works excellently on the first 13 observations. Since it is continuous, we can try to extrapolate it for some further time. As shown in Fig. 8.8, it works satisfactory up to 28 weeks (196 days).

Since at this time the hydraulic head nears the critical value 0.5, it may make no sense to extrapolate the obtained transforming mechanism further. As soon as the hydraulic head exceeds the critical value, new data should be collected for a new calibration. Let the collection start at week 30 and last for 13 weeks, i.e., during the period from days 210 to 301. The results of the model calibration are presented in Fig. 8.9 and seem to be satisfactory.

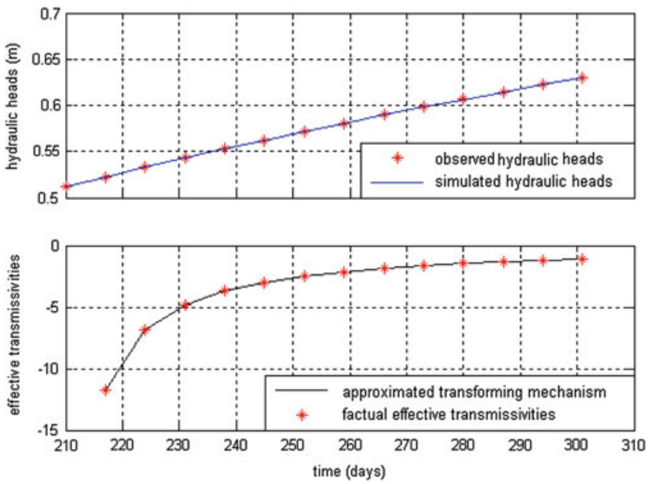


Fig. 8.9 Case 8.4.2: recalibration on data related to weeks 30–43

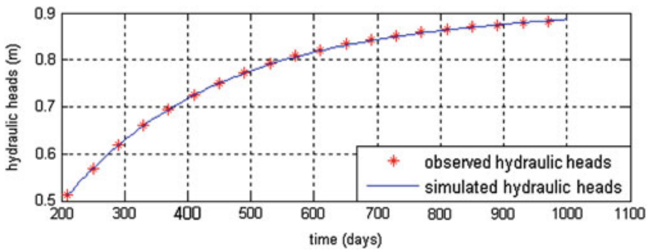


Fig. 8.10 Case 8.4.2: extrapolating simulations beyond period of calibration (43 weeks), applying the transforming mechanisms described by Eq. 8.25

The transforming mechanism in this case is represented by the regression

$$\frac{1}{\hat{T}} \approx -4.0923 \times 10^{-8}(t-\bar{t})^3 - 1.9219 \times 10^{-5}(t-\bar{t})^2 - 9.8878 \times 10^{-3}(t-\bar{t}) - 0.4697, \quad (8.25)$$

where $\bar{t} = 259$ days.

This transforming mechanism was extrapolated on all the remaining period of simulation for weeks 30–143 (about 1,000 days). As shown in Fig. 8.10, there is no need for model recalibration.

Contrary to in case 8.4.1, location $L = 50$ m is not a bad choice for monitoring this object, since the range of the hydraulic heads is larger in this case. The point here is that, when assuming different values T_1 and T_2 or rather different ratios T_2/T_1, the choice for location or locations for monitoring wells can be done prior to starting field explorations.

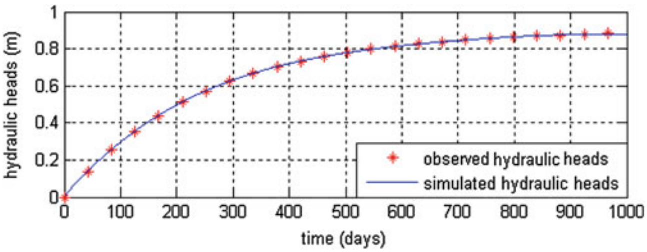


Fig. 8.11 Case 8.4.2: reproducing the development of hydraulic heads by Eq. 8.26 without involving effective hydraulic transmissivities

8.5 Conclusions

This chapter illustrates the general concept and demonstrates the possibility to evaluate the mechanisms transforming real properties of geological objects into the parameters which are effective in simulation of predictive or evaluative problems according to those problems' formulations. However, evaluating nonlinear transformations may face considerable computational difficulties.

Indeed, evaluation of linear transforming mechanisms is straightforward. If a linear mechanism depends on time, the procedure described in Sects. 8.1–8.2 must be repeated for the instants of interest. Moreover, this can be done before beginning field exploration. Evaluation of nonlinear mechanisms requires some knowledge on the object's reaction to the planned impact, that is, monitoring of the reaction, and model recalibration from time to time.

By the way, it is possible to predict the development of the hydraulic heads without finding effective parameters, transforming mechanisms, and physically based simulation models at all. The available observations can be used to evaluate the regression relationship describing those observations in time, which can then be extrapolated into the future. When this becomes unsatisfactory, the additional data obtained by monitoring are applied to obtain a new regression relationship, and so on. In particular, in case 8.4.2, the regression

$$\hat{h} \approx -1.66 \times 10^{-12} t^4 + 4.9846 \times 10^{-9} t^3 - 5.8572 \times 10^{-6} t^2 + 0.0034t \quad (8.26)$$

works satisfactorily (Figs. 8.10, 8.11).

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Chapter 9
Inverse Problems and Transforming Mechanisms

As mentioned in Chap. 4, the term "inverse problem" is not a synonym for the terms "model identification," "model calibration," "historical matching," or "site-specific validation." Those terms relate to evaluating the effective characteristics for a given simulation model, which is usually an optimization problem. The goal of the inverse problem is to estimate the actual properties of geological objects using available observations on natural geological phenomena or on responses on manmade impacts. Since the notions of geological objects are not more than models, it seems to be more accurate to define inverse problems as applications of simpler models for evaluating properties of more complex ones. The simpler models applied for solving inverse problems are called *interpretation models*.

The physical and geological meanings of the results of model identification do not matter. The effective parameters must provide the best results for the coupled simulation problem, and they depend on its formulation. In contrast, the result of solving an inverse problem must not depend on its formulation, and its solution is not acceptable if it is deprived of physical meaning.

As demonstrated in Sect. 6.3, the linear transforming mechanisms obtained in Sect. 6.2 can be applied to solve inverse problems in a straightforward way. Indeed, if affecting factors $w_{j,i}$ ($j = 1, 2$ indicates model blocks, $i = 1, 2, 3, 4$ geological bodies) and the pertinent effective parameters $\hat{g}_j$ are known, a transforming mechanism

$$w_{j,1}g_1 + w_{j,2}g_2 + w_{j,3}g_3 + w_{j,4}g_4 = \hat{g}_j \tag{9.1}$$

can be considered as an equation with respect to the unknown actual property values $g_{1...4}$. So, it suffices to make up a sufficient number of transforming mechanisms with known affecting factors and effective parameter values, to consider them as a system of equations, closed or redundant, and than to solve it for $g_{1...4}$. Exactly this has been done in Sect. 6.3 (system 6.24). However, the development of many different formulations of a model identification problem,

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_9,

such as those in Sect. 6.2, is a cumbersome enterprise. The approach described in this chapter permits making this procedure more practical. It is based on assigning different (random) sets of weights to the available observations.

Inverse problems are inherently incorrect. However, as shown in Sect. 4.1, this does not mean that they are incorrect always. The mathematical correctness or incorrectness of an inverse problem depends on the actual structure and properties of the geological object, the choice of the model representing the object, and the diversity and accuracy of the available observations. Any practicing geophysicist has the experience of success and failure of interpretation of geophysical data. Understanding the geology and the observed process are necessary conditions for success.

9.1 Linear Transforming Mechanisms: Illustrative Examples

Let us rewrite criterion 6.6, introducing arbitrary subsets of the weights $\{p\}_m = \{p_{m,1}\ p_{m,2},\ p_{m,3}\ p_{m,4}\}$ to the errors of our simulation of the squared thickness of the aquifer in different observation locations:

$$s_m = \sum_{i=1}^{4} p_{m,i}\left(\hat{h}_{p,i}^2 - h_i^2\right)^2. \tag{9.2}$$

Then system 6.10 converts into

$$\begin{aligned}
&\left(0.4375^2 p_{m,1} + 0.75^2(p_{m,2} + p_{m,3} + p_{p,4})\right)\hat{g}_{m,1} + 0.75(0.1875 p_{m,3} + 0.25 p_{m,4})\hat{g}_{m,2} \\
&\quad = 0.4375 p_{m,1}\left(h_1^2 - h_0^2\right) + 0.75\left(p_{m,2}\left(h_2^2 - h_0^2\right) + p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0^2\right)\right), \\
&0.75(0.1875 p_{m,3} + 0.25 p_{m,4})\hat{g}_{p,1} + \left(0.1875^2 p_{m,3} + 0.25^2 p_{m,4}\right)\hat{g}_{m,2} \\
&\quad = 0.1875 p_{m,3}\left(h_3^2 - h_0^2\right) + 0.25 p_{m,4}\left(h_4^2 - h_0^2\right).
\end{aligned} \tag{9.3}$$

The matrix of system (9.3) is

$$c_m = \begin{Bmatrix} 0.4375^2 p_{m,1} + 0.75^2(p_{m,2} + p_{m,3} + p_{m,4}) & 0.75(0.1875 p_{m,3} + 0.25 p_{m,4}) \\ 0.75(0.1875 p_{m,3} + 0.25 p_{m,4}) & 0.1875^2 p_{m,3} + 0.25^2 p_{m,4} \end{Bmatrix} \tag{9.4a}$$

The right-hand term vector is

$$b_m = \begin{Bmatrix} 0.4375 p_{m,1}\left(h_1^2 - h_0^2\right) + 0.75\left(p_{m,2}\left(h_2^2 - h_0^2\right) + p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0^2\right)\right) \\ 0.1875 p_{m,3}\left(h_3^2 - h_0^2\right) + 0.25 p_{m,4}\left(h_4^2 - h_0^2\right) \end{Bmatrix} \tag{9.4b}$$

(compare to expressions 6.11). Solving system (9.3) yields two values of the effective hydraulic resistivities: $\hat{g}_{2m-1}$ and $\hat{g}_{2m}$.

Table 9.1 Set consisting of M subsets of weights for evaluating the real-life hydraulic resistivities as regression coefficients

Eq. No.	Weights	Effective parameters	Affecting factors
1	$\{p\}_1$	$\hat{g}_{1,1}$	$\{w_{1,1,1}, w_{1,1,2}, w_{1,1,3}, w_{1,1,4}\}$
2		$\hat{g}_{1,2}$	$\{w_{1,2,1}, w_{1,2,2}, w_{1,2,3}, w_{1,2,4}\}$
3	$\{p\}_2$	$\hat{g}_{2,3}$	$\{w_{2,3,1}, w_{2,3,2}, w_{2,3,3}, w_{2,3,4}\}$
4		$\hat{g}_{2,4}$	$\{w_{2,4,1}, w_{2,4,2}, w_{2,4,3}, w_{2,4,4}\}$
…………	……..	…………………	………………………
$2m-1$	$\{p\}_m$	$\hat{g}_{m,2m-1}$	$\{w_{m,2m-1,1}, w_{m,2m-1,2}, w_{m,2m-1,3}, w_{\mathrm{m},2m-1,4}\}$
$2m$		$\hat{g}_{m,2m}$	$\{w_{\mathrm{m},2m,1}, w_{\mathrm{m},2m,2}, w_{\mathrm{m},2m,3}, w_{\mathrm{m},2m,4}\}$
…………	……..	…………………	………………………
$2M-1$	$\{p\}_M$	$\hat{g}_{M,2M-1}$	$\{w_{\mathrm{M},2M-1,1}, w_{\mathrm{M},2M-1,2}, w_{\mathrm{M},2M-1,3}, w_{\mathrm{M,2M-1,\ 4}}\}$
$2M$		$\hat{g}_{M,2M}$	$\{w_{\mathrm{M},2M,1}, w_{\mathrm{M},2M,2}, w_{\mathrm{M},2M,3}, w_{\mathrm{M},2M,4}\}$

To find the affecting factors of the corresponding transforming mechanisms, Eq. 6.15 can be applied to each set of weights:

$$\begin{aligned} \{\, w_{2m-1,1} \quad w_{2m-1,2} \quad w_{2m-1,3} \quad w_{2m-1,4} \,\} &= \left\{ \frac{W_{2m-1}c_{m,2,2} - W_{2m}c_{m,1,2}}{c_{m,1,1}c_{m,2,2} - c_{m,1,2}c_{m,2,1}} \right\}', \\ \{\, w_{2m,1} \quad w_{2m,2} \quad w_{2m,3} \quad w_{2m,4} \,\} &= \left\{ \frac{W_{2m,}c_{m,1,1} - W_{2m-1,1}c_{m,2,1}}{c_{m,1,1}c_{m,2,2} - c_{m,1,2}c_{m,2,1}} \right\}', \end{aligned} \tag{9.5}$$

where the vectors W_{2m-1} and W_{2m} are defined by expression 6.14,

$$\begin{aligned} W_{2m-1} &= \begin{Bmatrix} 0.4375\big(0.4375p_{m,1} + 0.75(p_{m,2} + p_{m,3} + p_{m,4})\big) \\ 0.3125 \times 0.75(p_{m,2} + p_{m,3} + p_{m,4}) \\ 0.1875 \times 0.75(p_{m,3} + p_{m,4}) \\ 0.75 \times 0.0625p_{p,4} \end{Bmatrix}, \\ W_{2m} &= \begin{Bmatrix} 0.4375(0.1875p_{m,3} + 0.25p_{m,4}) \\ 0.3125(0.1875p_{m,3} + 0.25p_{m,4}) \\ 0.1875(0.1875p_{m,3} + 0.25p_{m,4}) \\ 0.25 \times 0.0625p_{m,4} \end{Bmatrix}. \end{aligned} \tag{9.6}$$

Thus, in the case of a two-block interpretation model and M sets of weights $\{p\}_m$, we can accumulate $2M$ effective values and sets of affecting factors (Table 9.1), permitting making up of an excessive system for evaluating the four actual hydraulic resistivities g_1, g_2, g_3, g_4.

To solve the above excessive system, the least-squares method can be applied; that is, the unknown values g_1, g_2, g_3, g_4 are considered as the regression coefficients minimizing the sum

Table 9.2 "Observed" data in case 6.2.2

j	0	1	2	3	4
x (m)	0	25	50	75	100
$h^2(m^2)$	0.01	4.3850	5.9475	6.1558	6.2183

$$s_m = \sum_{m=1}^{2M} \left(g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} - \hat{g}_m\right)^2. \tag{9.7}$$

Applying the standard least-squares technique to sum 9.7 leads to the following system of four equations:

$$\begin{aligned}
&g_1 \sum_{m=1}^{2M} w_{m,1}^2 + g_2 \sum_{m=1}^{2M} w_{m,1} w_{m,2} + g_3 \sum_{m=1}^{2M} w_{m,1} w_{m,3} + g_4 \sum_{m=1}^{2M} w_{m,1} w_{m,4} = \sum_{m=1}^{2M} w_{m,1} \hat{g}_{m,1},\\
&g_1 \sum_{m=1}^{2M} w_{m,2} w_{m,1} + g_2 \sum_{m=1}^{2M} w_{m,2}^2 + g_3 \sum_{m=1}^{2M} w_{m,2} w_{m,3} + g_4 \sum_{m=1}^{2M} w_{m,2} w_{m,4} = \sum_{m=1}^{2M} w_{m,2} \hat{g}_{m,2},\\
&g_1 \sum_{m=1}^{2M} w_{m,3} w_{m,1} + g_2 \sum_{m=1}^{2M} w_{m,3} w_{m,2} + g_3 \sum_{m=1}^{2M} w_{m,3}^2 + g_4 \sum_{m=1}^{2M} w_{m,3} w_{m,4} = \sum_{m=1}^{2M} w_{w,3} \hat{g}_{m,3},\\
&g_1 \sum_{m=1}^{2M} w_{m,4} w_{m,1} + g_2 \sum_{m=1}^{2M} w_{m,4} w_{m,2} + g_3 \sum_{m=1}^{2M} w_{m,4} w_{m,3} + g_4 \sum_{m=1}^{2M} w_{m,4}^2 = \sum_{m=1}^{2M} \hat{g}_{m,4} w_{m,4}.
\end{aligned} \tag{9.8}$$

Solving the above system yields the values $g_{1\ldots4}$.

Case 9.1.1 Let the available observations on the squared water table elevations be those obtained and used in case 6.2.2. The squared elevations in Table 9.2 are obtained with the following distribution of hydraulic conductivities: $K_1 = 0.1$, $K_2 = 0.2$, $K_3 = 0.9$ and $K_4 = 1$ m/day in the intervals [0, 25], (25, 50], (50, 75], and (75, 100] m, respectively.

Applying the above procedure to the data presented in Table 9.2 with use of 100 transforming mechanisms ($M = 50$) yields

$$K_1 = 0.1000,\ K_2 = 0.2000, K_3 = 0.9001, K_4 = 1.0000 \text{ m/day};$$

that is, the above procedure solves the inverse problem accurately.

Since the inverse problem is prone to incorrectness, it is interesting to consider how the errors in the initial data affect the results. Thus, rounding the squared water table elevations in Table 9.2 to three digits after the decimal point results in the solution

$$K_1 = 0.1000, K_2 = 0.1999, K_3 = \ 0.9014, K_4 = 1.0081 \text{ m/day}.$$

Rounding the same data to two digits after the decimal point yields

$$K_1 = 0.0999,\ K_2 = 0.2003,\ K_3 = 0.8929,\ K_4 = 1.0417\,\text{m/day}.$$

Table 9.3 "Observed" data in case 6.2.1

Effective conductivity (m/day)	$\hat{K}_1 = 1.0011$		$\hat{K}_2 = 0.1678$		
x (m)	0	25	50	75	100
$h^2(m^2)$	0.4475	0.7947	1.7322	2.3572	0.4475

Rounding the same data to one digit after the decimal point results in

$$K_1 = 0.1,\; K_2 = 0.2,\; K_3 = 0.6,\; K_4 = 1.49 \times 10^{13}\text{m/day}.$$

This result, at least regarding K_4, is unacceptably corrupt. (The error in the value K_3 of about 30% could be considered as acceptable by many practitioners).

The last result demonstrates the incorrectness (instability) of this inverse problem. The reason is that the slope of the water table approaches the water divide at $x = 100$ m and becomes about horizontal: the difference between water table elevations at $x_3 = 75$ and $x_4 = 100$ m is less than 2 cm. This situation is close to that presented in Fig. 4.1. It is difficult to expect that, under such circumstances, there exists a mathematical manipulation able to convert the problem into a correct one. If it is impossible to improve the accuracy of the initial data, we have to exclude the data related to location x_4 from consideration and limit ourselves to finding the hydraulic conductivities K_1, K_2, and K_3. To evaluate the hydraulic conductivity of the fourth body, the aquitard must be perturbed by a pumping test or in some other way.

The data on case 6.2.2 were selected because reproducing the aquifer thicknesses is much worse than in case 6.2.1. Nevertheless, it is interesting to apply the above procedure to the data of case 6.2.1. The intervals with different values of the hydraulic conductivity in case 6.2.1 are the same as in case 6.2.2. The corresponding values of the conductivity are $K_1 = 1$, $K_2 = 0.9$, $K_3 = 0.2$, and $K_4 = 0.1$ m/day. The squared thicknesses of the aquifer for this case are presented in Table 9.3.

Application of the above-described procedure to the data in Table 9.3 yields the following results:

$$K_1 = 1.0000,\; K_2 = 0.9001,\; K_3 = 0.2000,\; K_4 = 0.1000\,\text{m/day}.$$

Rounding the squared water table elevations in Table 6.3 to three digits after the decimal point results in the solution

$$K_1 = 0.9989,\; K_2 = 0.9006,\; K_3 = 0.2001,\; K_4 = 0.1000\,\text{m/day}.$$

Rounding the same data to two digits after the decimal point yields

$$K_1 = 0.9943,\; K_2 = 0.9191,\; K_3 = 0.1995,\; K_4 = 0.0992\,\text{m/day}.$$

Rounding the same data to one digit after the decimal point results in

$$K_1 = 1.1218,\; K_2 = 0.7812,\; K_3 = 0.2083,\; K_4 = 0.0893\,\text{m/day}.$$

These results seem to be more stable and accurate due, probably, to the absence of "observations" which are not indistinguishable practically.

Case 9.1.2 Let the interpretational model be the simplest one, i.e., homogeneous. For this model the relationship between the effective hydraulic resistivity and the effective squared water table can be represented as follows:

$$\begin{aligned} \hat{h}_1^2 - h_0^2 &= 0.4375\hat{g} \\ \hat{h}_2^2 - h_0^2 &= 0.75\hat{g} \\ \hat{h}_3^2 - h_0^2 &= 0.9375\hat{g} \\ \hat{h}_4^2 - h_0^2 &= \hat{g} \end{aligned} \tag{9.9}$$

Criterion 9.2 takes the form

$$\begin{aligned} s_m = p_{m,1}\left(0.4375\hat{g}_m - \left(h_1^2 - h_0^2\right)\right)^2 + p_{m,2}\left(0.75\hat{g}_m - \left(h_2^2 - h_0^2\right)\right)^2 \\ + p_{m,3}\left(0.9375\hat{g}_m - \left(h_3^2 - h_0^2\right)\right)^2 + p_{m,4}\left(\hat{g}_m - \left(h_4^2 - h_0^2\right)\right)^2, \end{aligned} \tag{9.10}$$

where $\{p\}_m$ is the mth set of weights. Applying the standard least-squares technique yields

$$\hat{g}_m = \frac{0.4375p_{p,1}\left(h_1^2 - h_0^2\right) + 0.75p_{m,2}\left(h_2^2 - h_0^2\right) + 0.9375p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0^2\right)}{0.4375^2p_{m,1} + 0.75^2p_{m,2} + 0.9375^2p_{m,3} + p_{m,4}}. \tag{9.11}$$

The actual squared water table elevations are described by the expressions

$$\begin{aligned} h_1^2 - h_0^2 &= 0.4375g_1 \\ h_2^2 - h_0^2 &= 0.4375g_1 + 0.3125g_2 \\ h_3^2 - h_0^2 &= 0.4375g_1 + 0.3125g_2 + 0.1875g_3 \\ h_4^2 - h_0^2 &= 0.4375g_1 + 0.3125g_2 + 0.1875g_3 + 0.0625g_4 \end{aligned} \tag{9.12}$$

Substituting expression 9.12 in Eq. 9.11 and combining the terms containing the same real-world hydraulic resistivities yields the following affecting factors:

$$\begin{aligned} w_{m,1} &= \frac{0.4375(0.4375p_{m,1} + 0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4})}{c_m} \\ w_{m,2} &= \frac{0.3125(0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4})}{c_m} \\ w_{m,3} &= \frac{0.1875(0.9375p_{m,3} + p_{m,4})}{c_m} \\ w_{m,4} &= \frac{0.0625p_{m,4}}{c_m}, \end{aligned} \tag{9.13}$$

where

$$c_m = 0.4375^2 p_{m,1} + 0.75^2 p_{m,2} + 0.9375^2 p_{m,3} + p_{m,4}. \tag{9.14}$$

Thus, we obtain regression 9.1

$$g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} = \hat{g}_m \tag{9.15}$$

and find the pertinent hydraulic resistivities as coefficients of the above regression in which the affecting factors $w_{m,i}$ play the role of independent variables and $\hat{g}_m$ is calculated based on the observations.

The homogeneous model yields results which are exactly the same as in case 9.1.1, though the model and the inverse problem solving are considerably simpler.

Case 9.1.3 Cases 9.1.1 and 9.1.2 demonstrated that the transforming mechanisms can be successfully applied for inverse problem solving in some situations. However, this is not always so. Let us now assume that, in the inverse problem considered above, the geological object consists of eight geological bodies with boundaries at locations $X_0 = 0$, $X_1 = 12.5$, $X_2 = 25$, $X_3 = 37.5$, $X_4 = 50$, $X_5 = 62.5$, $X_6 = 75$, $X_7 = 87.5$, and $X_8 = 100$ m, with constant hydraulic conductivities within the intervals $[X_{j-1}, X_j]$: K_1, K_2, K_3, K_4, K_5, K_6, K_7, and K_8 (hydraulic resistivities $g_1 = 1/K_1$, $g_2 = 1/K_2$, $g_3 = 1/K_3$, $g_4 = 1/K_4$, $g_5 = 1/K_5$, $g_6 = 1/K_6$, $g_7 = 1/K_7$, and $g_8 = 1/K_8$). The monitoring network and the observed squared water table elevations are those presented in Table 9.2. The recharge rate also remains the same, $N = 0.0001$ m/day. The task is to find the hydraulic conductivities K_1, K_2, K_3, K_4, K_5, K_6, K_7, and K_8 based on the available water table elevations using a homogeneous interpretation model.

The approach to solving this inverse problem remains the same as in the previous cases. Namely, the unknown hydraulic resistivities g_1 to g_8 are coefficients of the linear regression

$$g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} + g_5 w_{m,5} + g_6 w_{m,6} + g_7 w_{m,7} + g_8 w_{m,8} = \hat{g}_m, \tag{9.16}$$

where $w_{m,i}$ ($i = 1$–8) are the pertinent affecting factors corresponding to the set of weights $\{p\}_m = \{p_{m,1}, p_{m,2}, p_{m,3}, p_{m,4}\}$ and playing the role of independent variables; $\hat{g}_m$ is the known pertinent effective value of the hydraulic resistivity, the "observation." Thus, the goal is to make up a large number of sets of the affecting factors $\{w\}_m = \{w_{m,1}, w_{m,2}, \ldots, w_{m,8}\}$ and the pertinent effective parameters $\hat{g}_m$.

The effective resistivity $\hat{g}_m$ corresponding to the set of weights $\{p\}_m = \{p_{m,1}, p_{m,2}, p_{m,3}, p_{m,4}\}$ can be calculated by Eq. 9.9. In the case of the eight-body real world, Eq. 9.10 becomes

$$\begin{aligned}
h_1^2 - h_0^2 &= 0.2344g_1 + 0.2031g_2 \\
h_2^2 - h_0^2 &= 0.2344g_1 + 0.2031g_2 + 0.1791g_3 + 0.1406g_4 \\
h_3^2 - h_0^2 &= 0.2344g_1 + 0.2031g_2 + 0.1791g_3 + 0.1406g_4 + 0.1094g_5 + 0.0781g_6 \\
h_4^2 - h_0^2 &= 0.2344g_1 + 0.2031g_2 + 0.1791g_3 + 0.1406g_4 + 0.1094g_5 + 0.0781g_6 \\
&\quad +0.0469g_7 + 0.01563g_8
\end{aligned} \tag{9.17}$$

Substituting expression 9.17 in Eq. 9.11 and calculating multipliers in terms with different $g_{1\ldots8}$ yields the following affecting factors

$$\begin{aligned}
w_{m,1} &= \frac{0.2344(0.4375p_{m,1} + 0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4})}{c_m}; & w_{m,2} &= \frac{0.2031w_{m,1}}{0.2344} \\
w_{m,3} &= \frac{0.1719(0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4})}{c_m}; & w_{m,4} &= \frac{0.1406w_{m,3}}{0.1719} \\
w_{m,5} &= \frac{0.1094(0.9375p_{m,3} + p_{m,4})}{c_m}; & w_{m,6} &= \frac{0.0781w_{m,4}}{0.1094} \\
w_{m,7} &= \frac{0.0469p_{m,4}}{c_m}; & w_{m,8} &= \frac{0.01563p_{m,4}}{0.0469}
\end{aligned} \tag{9.18}$$

where the denominator c_m is defined by Eq. 9.14.

Now we can apply the standard least-squares technique to evaluate the unknown hydraulic resistivities $g_{1\ldots8}$, the regression coefficients of regression 9.16. Based on the data presented in Table 9.2 and $M = 100$ corresponding to 100 sets of independent variables $\{w\}_m$ and the known values $\hat{g}_m$ we obtain

$$\begin{aligned}
K = [&-0.0321 \quad 0.0262 \quad -0.0596 \quad 0.0435 \\
&0.0848 \quad -0.2215 \quad -0.0021 \quad 0.0007\,]\ \text{m/day}
\end{aligned}$$

instead of the factual hydraulic conductivities

$$K = 0.\,1,\ 0.1,\ 0.2,\ 0.2,\ 0.9,\ 0.9,\ 1,\ 1\,\text{m/day}.$$

Thus, the inverse problem formulation in case 9.1.3 is incorrect. The mathematical cause of the incorrectness is poor conditioning of the system for finding the hydraulic resistivities $g_{1\ldots8}$. This happened because the affecting factors are mutually dependent and not sufficiently diverse. (This is not the case for evaluating the affecting factors per se by two-level modeling. Indeed, we are free to select any values of the real-world parameters and to make them as diverse as we want). However, the main reason is the mismatch of the complexity of the object and the data for solving the inverse problem. What may provide some comfort is the possibility to establish the correctness or incorrectness of the formulation of an inverse problem before starting field explorations through use of two-level modeling and to look for appropriate changes to the methodology of the investigations.

Table 9.4 Data for solving inverse problems for the Borden landfill

No.	x	H	$v = H - Y$	Y	H_S	$u = H_S - Y$	Q
0	300	222.31	17.99	204.31	222.31	17.99	Q_S
1	400	222.23	16.06	206.17	219.25	13.08	$Q_S + 100N_3$
2	500	222.11	12.56	209.55	218.26	8.71	$Q_S + 200N_3$
3	600	221.95	11.09	210.85	217.46	6.61	$Q_S + 300N_3$
4	700	221.72	10.39	211.33	216.07	4.74	$Q_S + 300N_3 + 100N_4$
5	800	221.42	9.56	211.86	215.47	3.61	$Q_S + 300N_3 + 200N_4$
6	900	221.04	8.24	212.79	215.67	2.88	$Q_S + 300N_3 + 200N_4 + 100N_5$

9.2 Borden Landfill: Evaluating Actual Recharge Rates

Let the simulation model in Sect. 4.4 represent the real geological object accurately. The goal is to evaluate the actual recharge rates pertaining to the intervals (300, 600], (600, 800], and (800, 900] m assigned by Frind and Hokkanen (1987). The data for solving the inverse problems are presented in Table 9.4 (cf. Tables 6.11 and 6.12). They comprise the available observations on the water table and the streamline starting at $x = 300$ m and the expressions for calculating the total flux at the points of observations. (The recharge rates in the interval [0, 300] m and the total flux $Q_S = Q(300) = 0.1253$ m^2/day are assumed known).

Case 9.2.1 Let the interpretation model be homogeneous with respect to the recharge pattern for $x > 300$ m (Fig. 9.1). The approach to solving this inverse problem is roughly the same as in the previous section. Namely, the goal is to make up a manifold of transforming mechanisms by applying different subsets of weights to the observed data, $u_{1\ldots6}$. As soon as the manifold is obtained, the corresponding transforming mechanisms

$$N_3 w_{m,1} + N_4 w_{m,2} + N_5 w_{m,3} = \hat{N}_m \tag{9.19}$$

are considered as linear regressions with unknown regression coefficients $N_{3\ldots5}$. The effective recharge rates $\hat{N}_m$, corresponding to the random set of weights $\{p_{m,1\ldots6}\}$, can be evaluated based on the available observations. With all necessary data accumulated, the unknown recharge rates $N_{3\ldots5}$ can be obtained by standard least-squares technique by solving the following system:

$$\begin{aligned}
N_3 \sum_{m=1}^{M} w_{m,1}^2 + N_4 \sum_{m=1}^{M} w_{m,1} w_{m,2} + N_5 \sum_{m=1}^{M} w_{m,1} w_{m,3} &= \sum_{m=1}^{M} w_{m,1} \hat{N}_m \\
N_3 \sum_{m=1}^{M} w_{m,2} w_{m,1} + N_4 \sum_{m=1}^{M} w_{m,2}^2 + N_5 \sum_{m=1}^{M} w_{m,2} w_{m,3} &= \sum_{m=1}^{M} w_{m,2} \hat{N}_m \\
N_3 \sum_{m=1}^{M} w_{m,3} w_{m,1} + N_4 \sum_{m=1}^{M} w_{m,3} w_{m,2} + N_5 \sum_{m=1}^{M} w_{m,3}^2 &= \sum_{m=1}^{M} w_{m,3} \hat{N}_m
\end{aligned} \tag{9.20}$$

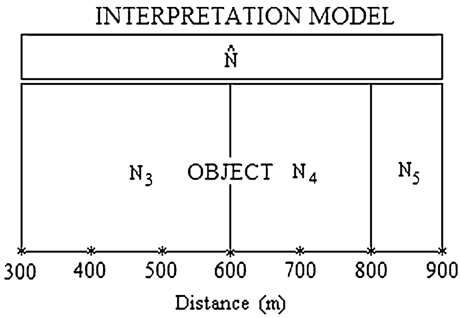

Fig. 9.1 Case 9.2.1: homogeneous interpretational model for evaluating recharge rates N_3, N_4, and N_5

In Sect. 6.4, the transforming mechanism was obtained analytically for uniform weighting. The same can be done for nonuniform weighting. Let us assume that recharges N_3, N_4, and N_5 are known. The effective recharge rates corresponding to the weighting $\{p_{m,\ 1\ldots6}\}$ and the above recharge pattern can be obtained straightforwardly by minimizing the criterion

$$s_m = \sum_{i=1}^{6} p_{m,i}\left(\hat{Q}_{m,i} - Q_i\right)^2 u_i^2, \tag{9.21}$$

where Q_i and $\hat{Q}_{m,i}$ are the actual and effective total fluxes at the observation points, presented in Table 9.5. The standard least-squares procedure requires solving the equation

$$\sum_{i=1}^{6} p_{m,i} u_i^2 \left(\hat{Q}_{m,i} - Q_i\right) \frac{\mathrm{d}\hat{Q}_{\mathrm{m,i}}}{\mathrm{d}\hat{N}_m} = 0. \tag{9.22}$$

Substituting in Eq. 9.22 the expressions for Q_i and $\hat{Q}_{m,i}$ from Table 9.5 and solving it for $\hat{N}_m$ yields Eq. 9.19, in which

$$w_{m,1} = b_{m,1}/c_m, \quad w_{m,2} = b_{m,2}/c_m, \quad w_{m,3} = b_{m,3}/c_m, \tag{9.23}$$

and

$$\begin{aligned} c_m &= p_{m,1}u_1^2 + 4p_{m,2}u_2^2 + 9p_{m,3}u_3^2 + 16p_{m,4}u_4^2 + 25p_{m,5}u_5^2 + 36p_{m,6}u_6^2 \\ b_{m,1} &= p_{m,1}u_1^2 + 4p_{m,2}u_2^2 + 9p_{m,3}u_3^2 + 12p_{m,4}u_4^2 + 15p_{m,5}u_5^2 + 18p_{m,6}u_6^2 \\ b_{m,2} &= 4p_{m,4}u_4^2 + 10p_{m,5}u_5^2 + 12p_{m,6}u_6^2 \\ b_{m,3} &= 6p_{m,6}u_6^2 \end{aligned} \tag{9.24}$$

(It is easy to check that, as expected, the affecting factors in mechanism 9.23 sum to one.)

Thus, the affecting factors comprising the coefficients of system 9.20 are obtained. To complete the creation of system (9.20), it is necessary to obtain the right-hand terms including $\hat{N}_m$, the actual effective recharge rates corresponding to different sets of weights $\{p_{m,\ 1\ldots6}\}$. They can be found by minimization of the criterion

Table 9.5 Case 9.2.1: expressions for calculating total fluxes Q_i and $\hat{Q}_{m,i}$

No.	x	Q	$\hat{Q}_m$
0	300	Q_S	Q_S
1	400	$Q_S + 100N_3$	$Q_S + 100\hat{N}_m$
2	500	$Q_S + 200N_3$	$Q_S + 200\hat{N}_m$
3	600	$Q_S + 300N_3$	$Q_S + 300\hat{N}_m$
4	700	$Q_S + 300N_3 + 100N_4$	$Q_S + 400\hat{N}_m$
5	800	$Q_S + 300N_3 + 200N_4$	$Q_S + 500\hat{N}_m$
6	900	$Q_S + 300N_3 + 200N_4 + 100N_5$	$Q_S + 600\hat{N}_m$

$$s_m = \sum_{i=1}^{6} p_{m,i}\left(\hat{Q}_{m,i}u_i - Q_S v_i\right)^2. \tag{9.25}$$

(cf. criterion 6.39). They are solutions of the equations

$$\begin{aligned}&100\left(p_{m,1}u_1^2 + 4p_{m,2}u_2^2 + 9p_{m,3}u_3^2 + 16p_{m,4}u_4^2 + 25p_{m,5}u_5^2 + p_{m,6}u_6^2\right)\hat{N}_1\\ &= Q_S\left(\begin{aligned}p_{m,1}u_1(v_1-u_1) + 2p_{m,2}u_2(v_2-u_2) + 3p_{m,3}u_3(v_3-u_3) + 4p_{m,4}u_4(v_4-u_4)\\ +5p_{m,5}u_5(v_5-u_5) + 6p_{m,6}u_6(v_6-u_6)\end{aligned}\right).\end{aligned} \tag{9.26}$$

Substituting the data from Tables 9.4 and 9.5 in Eq. 9.26 yields

$$\hat{N}_m = \frac{Q_S}{100}\frac{\sum_{i=1}^{6} p_{m,i}iu_i(v_i - u_i)}{\sum_{i=1}^{6} p_{m,i}i^2u_i^2}, \quad \left(Q_S = 0.1253\,\text{m}^2/\text{ day}\right). \tag{9.27}$$

Now, system 9.20 can be made up and solved. The results of several realizations of the above procedure are presented in Table 9.6. They seem consistent. The results obtained for $M = 50$ are presented in Fig. 9.2. They are practically satisfying: the travel time to $x = 900$ and 950 m is about 38.9 and 40 years. The magnitude of the maximal error in reproducing the streamline occurs at $x = 500$ m. It is less than 5 cm, which is better than that obtained in the process of model identification (Sect. 4.4). However, for $x > 800$ m the error grows considerably, meaning that the recharge rate N_5 needs correction. Besides, the condition numbers of system 9.20 for different M are large.

Fortunately, the interpretation model permits manual correction. Indeed, the model is such that the recharge rate N_5 for $x > 800$ m does not affect the previous observations. Thus, the recharge pattern

$$N_3 = 10.29, N_4 = 22.75 \text{ and } N_5 = 8\,\text{cm/year}$$

makes the magnitude of the error at $x = 900$ m close to 2 cm (compare with $N_3 = 10.2$, $N_4 = 23$, and $N_5 = 8.36$ cm/year in Table 4.4). The travel times to $x = 900$ and 950 m are about 39 and 40.2 years.

Table 9.6 Some results of solving the inverse problem in case 9.2.1 (M is the number of simulations)

M	Recharge rates (cm/year)			Condition number
	N_3	N_4	N_5	
10	10.38	22.53	16.70	6,017
50	10.29	22.75	18.33	4,261
250	10.31	22.68	18.89	3,992
1,250	10.30	22.68	18.59	4,247
6,250	10.30	22.66	18.66	3,897

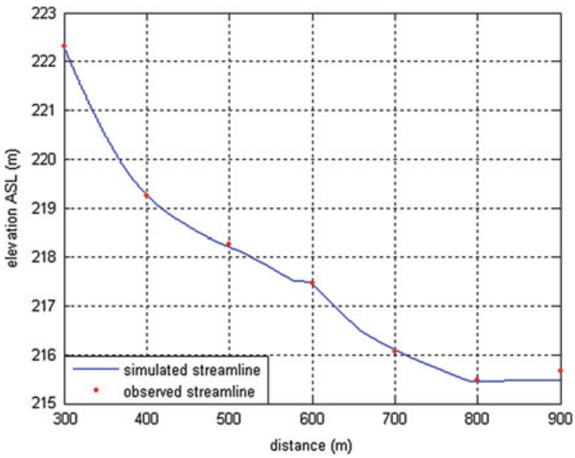

Fig. 9.2 Case 9.2.1: reproducing the streamline starting at $x = 300$ m using the recharge rates yielded by inverse problem solving

Case 9.2.2 Let us change the interpretation model. Now, it comprises two blocks: intervals (300, 600] m constitutes the first homogeneous block with effective recharge rate $\hat{N}_1$, and the interval (600, 900] m the second one with recharge rate $\hat{N}_2$ (Fig. 9.3).

In general, the procedure for solving the inverse problem in this case does not differ from the previous one. The goal is to create and solve a system of equations like system 9.20. The available information remains the same (Table 9.4), but two effective recharge rates now exist: $\hat{N}_{m,1}$ for the first model block and $\hat{N}_{m,2}$ for the second one in this case. They correspond to two different transforming mechanisms:

$$\begin{aligned}\hat{N}_{m,1} &= w_{m,1,1}N_3 + w_{m,1,2}N_4 + w_{m,1,3}N_5,\\ \hat{N}_{m,2} &= w_{m,2,1}N_3 + w_{m,2,2}N_4 + w_{m,2,3}N_5.\end{aligned} \tag{9.28}$$

The necessity to work with two transforming mechanisms could complicate the problem. In this case, it is not so. According to properties 1 and 2 of the transforming mechanisms (Sect. 5.3), the affecting factors $w_{m,1,1} = 1$, $w_{m,1,2} = -w_{m,1,3}$, $w_{m,2,1} = 0$, $w_{m,2,3} = 1 - w_{m,2,2}$ and mechanism 9.28 can be rewritten as

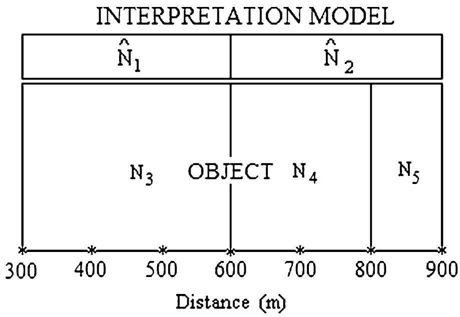

Fig. 9.3 Case 9.2.2: two-block interpretation model for finding recharge rates N_3, N_4, and N_5

$$\begin{aligned}\hat{N}_{m,1} &= N_3 + w_{m,1,2}N_4 - w_{m,1,2}N_5,\\ \hat{N}_{m,2} &= w_{m,2,2}N_4 + (1 - w_{m,2,2})N_5.\end{aligned} \tag{9.29}$$

However, we will consider all affecting factors as unknown and use their properties to the calculation.

Mechanism 9.28 can be evaluated analytically as was done in case 9.2.1, though this may be a cumbersome task. We come back to the standardized procedure described in Sects. 8.1–8.3. Let us assign R sets of recharge rates $\{rN_{r,3}, rN_{r,4}, rN_{r,5}\}$ at random. Then, for a given set of weights $\{p_{m,1\ldots6}\}$ and each set $\{rN_{r,3\ldots5}\}$, the effective recharge rates $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$ are evaluated by minimization of the criterion (cf. criterion 9.26)

$$s_{m,r} = \sum_{i=1}^{6} p_{m,i}u_i^2\left(\hat{Q}_{m,r,i} - Q_{r,i}\right)^2, \tag{9.30}$$

where u_i is the observed thickness of the aquifer's part below the streamline S, and expressions for calculating the effective total fluxes $\hat{Q}_{m,r,1}$ are presented in Table 9.7. The standard least-squares method leads to a system of two equations

$$\sum_{i=1}^{6} p_{m,i}u_i^2\left(\hat{Q}_{m,r,i} - Q_{r,i}\right)\frac{\hat{Q}_{m,r,i}}{\hat{N}_{m,r,j}}, \quad j = 1,\, 2, \tag{9.31}$$

which can be represented explicitly as

$$\begin{aligned}&\left(\sum_{i=1}^{3} i^2 p_{m,i}u_i^2 + 9\sum_{i=4}^{6} p_{m,i}u_i^2\right)\hat{N}_{m,r,1} + 3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2\right)\hat{N}_{m,r,2}\\ &= \left(\sum_{i=1}^{2} i^2 p_{m,i}u_i^2 + 9\sum_{i=3}^{6} p_{m,i}u_i^2\right)rN_3 + 3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2 - p_{m,6}u_i^2\right)rN_4 + 3p_{m,6}u_6^2 rN_5,\\ &3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2\right)\hat{N}_{m,r,1} + \left(\sum_{i=4}^{6}(i-3)^2 p_{m,i}u_i^2\right)\hat{N}_{m,r,2} = 3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2\right)rN_3\\ &\qquad + \left(p_{m,4}u_4^2 + 4p_{m,5}u_5^2 + 6p_{m,6}u_6^2\right)rN_4 + 3p_{m,6}u_6^2 rN_5.\end{aligned} \tag{9.32}$$

Table 9.7 Case 9.2.2: expressions for calculating total fluxes $Q_{r,i}$ and $\hat{Q}_{m,r,i}$

No.	x	Q_r	$\hat{Q}_{m,r}$
0	300	Q_S	Q_S
1	400	$Q_S + 100\mathrm{N}_{\mathrm{r},3}$	$Q_S + 100\hat{N}_{m,r,1}$
2	500	$Q_S + 200\mathrm{N}_{\mathrm{r},3}$	$Q_S + 200\hat{N}_{m,r,1}$
3	600	$Q_S + 300\mathrm{N}_{\mathrm{r},3}$	$Q_S + 300\hat{N}_{m,r,1}$
4	700	$Q_S + 300\mathrm{N}_{\mathrm{r},3} + 100\mathrm{N}_{\mathrm{r},4}$	$Q_S + 300\hat{N}_{m,r,1} + 100\hat{N}_{m,r,2}$
5	800	$Q_S + 300\mathrm{N}_{\mathrm{r},3} + 200\mathrm{N}_{\mathrm{r},4}$	$Q_S + 300\hat{N}_{m,r,1} + 200\hat{N}_{m,r,2}$
6	900	$Q_S + 300\mathrm{N}_{\mathrm{r},3} + 200\mathrm{N}_{\mathrm{r},4} + 100\mathrm{N}_{\mathrm{r},4}$	$Q_S + 300\hat{N}_{m,r,1} + 300\hat{N}_{m,r,2}$

Solving system 9.32 yields M coupled values of the effective recharge rates $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$.

Substituting values $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$ in Eq. 9.28, which for fixed m and different r can be rewritten as

$$\begin{aligned}\hat{N}_{m,r,1} &= w_{m,1,1}rN_{r,3} + w_{m,1,2}rN_{r,4} + w_{m,1,3}rN_{r,5},\\ \hat{N}_{m,r,2} &= w_{m,2,1}rN_{r,3} + w_{m,2,2}rN_{r,4} + w_{m,2,3}rN_{r,5},\end{aligned} \tag{9.33}$$

we obtain the excessive system of linear equations for evaluating the unknown affecting factors $w_{m,j,1\ldots3}$ ($j = 1, 2$) by the least-squares method.

The next step is to evaluate the actual effective values $\hat{N}_{m,1}$ and $\hat{N}_{m,2}$ corresponding to different sets of weights applying the data from Tables 9.4 and 9.7 by minimization of criterion 9.25

$$\begin{aligned}&\left(p_{m,1}u_1^2 + 4p_{m,2}u_2^2 + 9\sum_{i=3}^{6}p_{m,i}u_i^2\right)\hat{N}_{m,1} + 3\sum_{i=4}^{6}p_{m,i}(i-3)u_i^2\hat{N}_{m,2}\\ &= \frac{Q_S}{100}\left(p_{m,1}u_1(v_1-u_1) + 2p_{m,2}u_2(v_2-u_2) + 3\sum_{i=3}^{6}p_{m,i}u_i(v_i-u_i)\right)\\ &3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2\right)\hat{N}_1 + \left(\sum_{i=4}^{6}(i-3)^2p_{m,i}u_i^2\right)\hat{N}_2 = \frac{Q_S}{100}\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i(v_i-u_i)\right).\end{aligned} \tag{9.34}$$

Its solution is $2M$ values of the effective recharge rates $\hat{N}_{m,1}$ and $\hat{N}_{m,2}$.

Now, the system of equations similar to system 9.20 can be made up and solved. Several results of realization of the above procedure are presented in Table 9.8. They are close to those obtained in case 9.2.1. Note that the condition number of system 9.20 in case 9.2.2 is much better then in case 9.2.1, meaning that the inverse problem in case 9.2.2 is practically stable.

Case 9.2.3 Let the interpretation model be an exact copy of the real object. This means that now for $x > 300$ m it comprises three blocks in the intervals [300, 600], [600, 800], and $x > 800$ m. In this case the above approach, that is, creating and solving systems of equations like system 9.19, does not work. Indeed, the three

Table 9.8 Some results of solving the inverse problem in case 9.2.2 (M is the number of simulations)

M	Recharge rates (cm/year)			Condition number
	N_3	N_4	N_5	
10	10.34	22.48	19.69	343
50	10.34	22.44	18.93	132
250	10.31	22.59	18.85	151
1,250	10.32	22.64	18.98	139
6,250	10.31	22.60	18.93	134

Table 9.9 Results of solving the inverse problem in case 9.2.3

Recharge rates (cm/year)			Condition number
N_3	N_4	N_5	
10.31	22.64	18.98	254

corresponding transforming mechanisms do not depend on weighting the observations, and the affecting factors stay the same: $w_{1,1} = w_{2,2} = w_{3,3} = 1$ and $w_{1,2} = w_{1,3} = w_{2,1} = w_{2,3} = w_{3,1} = w_{3,2} = 0$ for any weighting. This converts the current inverse problem into an optimization one: three unknown recharge rates N_3, N_4, and N_5 can be evaluated as the effective ones by straightforward application of the least-squares method, that is, by minimization of the criterion

$$s = \sum_{i=1}^{6} (Q_i u_i - Q_S v_i)^2, \tag{9.35}$$

where the total flux Q_i is defined by column $Q_{r,i}$ in Table 9.9 (index r ignored). The standard least-squares technique leads to the following system of linear equations:

$$\sum_{i=1}^{6} (Q_i u_i - Q_S v_i) u_i \frac{\mathrm{dQ_i}}{\mathrm{d}N_j} = 0, \quad j = 1,\ 2,\ 3, \tag{9.36}$$

which can be presented explicitly as

$$\begin{aligned}
&\left(\sum_{i=1}^{3} i^2 u_i^2 + 9\sum_{i=4}^{6} u_i^2\right) N_3 + 3\left(u_4^2 + 2u_5^2 + 2u_6^2\right) N_4 + 3u_6^2 N_5 \\
&\quad = \tfrac{Q_S}{100}\left(u_1(v_1 - u_1) + 2u_2(v_2 - u_2) + 3\sum_{i=3}^{6} u_i(v_i - u_i)\right) \\
&3\left(u_4^2 + 2u_5^2 + 2u_6^2\right) N_3 + \left(u_4^2 + 4u_5^2 + 4u_6^2\right) N_4 + 2u_6^2 N_5 \\
&\quad = \tfrac{Q_S}{100}\left(u_4(v_4 - u_4) + 2u_5(v_5 - u_5) + 2u_6(v_6 - u_6)\right) \\
&3u_6^2 N_3 + 2u_6^2 N_4 + u_6^2 N_5 = \tfrac{Q_S}{100} u_6(v_6 - u_6)
\end{aligned} \tag{9.37}$$

The results of solving system 9.37 are presented in Table 9.9. They are close to the results obtained in cases 9.2.1 and 9.2.2.

The overestimation of the rate N_5 with respect to the effective value $\hat{N}_5$ may cause some discomfort, though the difference between them can be considered as acceptable practically. The reason is the same: too many assumptions, in particular about the structure of the real object and the steady-state water table. However, different formulations of the considered inverse problem led to consistent results. This could be a good reason to reconsider the assumptions applied in the model identification.

9.3 Nonlinear Transforming Mechanisms: Illustrative Example

Conceptually, solving inverse problems involving nonlinear transforming mechanisms does not differ from solving inverse problems involving linear ones, although technically they can be considerably more complicated. However, those problems can be solved, especially for not very complex real worlds. Interpretation of apparent resistance obtained by vertical electric sounding is an obvious example. The following conceptual example demonstrates, at least in principle, the possibility of formulation of and solving the hydrogeological inverse problem by applying the effective, or rather apparent, parameters.

Let us come back to the object presented first in Sect. 4.3, that is, a confined aquifer comprising two homogeneous bodies having hydraulic transmissivities T_1 and T_2 (Fig. 9.4). In the initial state the aquifer has uniform distributions of hydraulic heads $h(x, 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L = 100$ m jumps instantly to $h(2L, 0) = H_{2L}$ and stays the same: $h(2L, t) = H_{2L}$. At $x = 0$ the hydraulic head does not change: $h(0, t) = H_0$. (Without loss of generality, the values H_0 and H_{2L} are assigned equal to 0 and 1 m.) The jump of the hydraulic head at $x = 2L$ initiates the process of changing the aquifer hydraulic heads. The goal is to evaluate the hydraulic conductivities, observing the changing hydraulic head $h(L, t)$ at $x = L = 50$ m and using a homogeneous, one-block, interpretational model.

The transforming mechanism acting in this problem is described by Eq. 7.13, which is presented here for convenience

$$\hat{T}_i = -\frac{h_{i-1}}{1 - 2h_{i-1}} T_1 + \frac{1 - h_{i-1}}{1 - 2h_{i-1}} T_2, \tag{9.38}$$

where $h_{i\text{-}1} = h(L, t_{i-1})$. In terms of the affecting factors $w_{i,1}$ and $w_{i,2}$, Eq. 9.38 can be rewritten as

$$\hat{T}_i = T_1 w_{1,i} + T_2 w_{2,i}, \tag{9.39}$$

where

$$w_{1,i} = -\frac{h_{i-1}}{1 - 2h_{i-1}} \text{ and } w_{2,i} = \frac{1 - h_{i-1}}{1 - 2h_{i-1}}. \tag{9.40}$$

The simplest way of solving the inverse problem is to consider Eq. 9.39 for two different instants t_i and t_j and solve the system of these two equations.

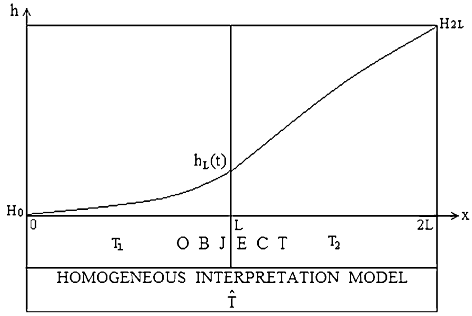

Fig. 9.4 Two-body object and homogeneous interpretation model (confined aquifer with horizontal base)

Equation 9.39 can be interpreted also as a linear regression with T_1 and T_2 as unknown actual transmissivities and one of the affecting factors as the independent variable ($w_{1,i} = 1 - w_{2,i}$). T_1 and T_2 can be found by the least-squares method exactly in the same way as was done in the cases above with the linear transforming mechanisms. Several results of solving inverse problems based on regression 9.39 are presented in Table 9.10. The corresponding forward problems, providing "observations," are produced explicitly (Sect. 7.2). Since the method of simulations is explicit, the time increment is chosen to be small, $\Delta t = 0.1$ days. In solving the corresponding inverse problems, the observations are made once a day, once a week, and once in 2 weeks. The period of observation is chosen as 182 days to avoid the instant of possible discontinuity of the transforming mechanisms when $T_1 < T_2$ as discussed in case 7.2.2.

There are many other ways of solving this simple inverse problem; for example, it follows from Eq. 9.38 that $\hat{T}_{i-1,i} = T_2$ for $h_{i-1} = 0$. This fact can be helpful also. On the other hand, the observed $h(t)$ at $x = L$ have a limit described by Eq. 4.31. For $H_0 = 0$ and $H_{2L} = 1$, Eq. 4.31 becomes

$$H_L = \frac{T_2}{T_1 + T_2}. \tag{9.41}$$

Correspondingly,

$$T_1 = \frac{1 - H_L}{H_L} T_2. \tag{9.42}$$

It may not be necessary to use transforming mechanisms to solve inverse problems; rather, one can operate with the effective transmissivity directly. The curves of effective transmissivity versus time for once-a-week observations are presented in Figs. 9.5 and 9.6. (Such curves are called master curves in geophysics).That is, the factual curve obtained based on actual observations can be compared with the master curves: the master curve best fitting the observations provides the transmissivity T_1. (The transmissivity T_2 can be evaluated as the left asymptote of the curves).

Such an approach is typical in applied geophysics, and for vertical electric sounding in particular. Indeed, apparent electric resistivities are actually effective

Table 9.10 Solving inverse problems by regression 9.39

Actual transmissivity (m^2/day)		Interval between measurements (days)					
		1		7		14	
T_1	T_2	Results of solving inverse problems: T_1, T_2 (m^2/day)					
0.1	0.9	0.1050	0.9013	0.1050	0.9013	0.1056	0.9016
0.5	0.9	0.5005	0.8999	0.5005	0.8999	0.5006	0.8999
0.9	0.9	0.9000	0.9000	0.9000	0.9000	0.9000	0.9000
0.9	0.5	0.9000	0.5001	0.9000	0.5001	0.9000	0.5001
0.9	0.1	0.9003	0.1000	0.9003	0.1000	0.9003	0.1000

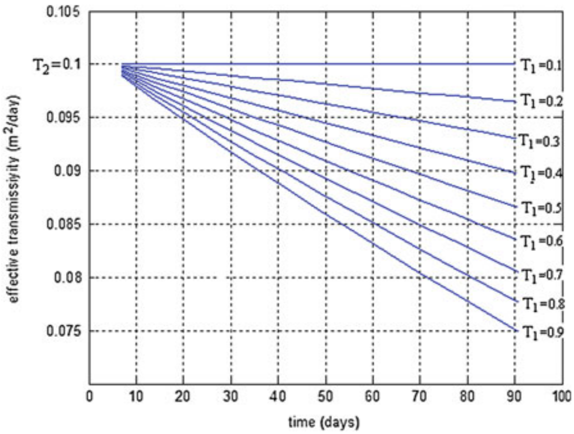

Fig. 9.5 Master curves for effective transmissivities for $T_2 < T_1$

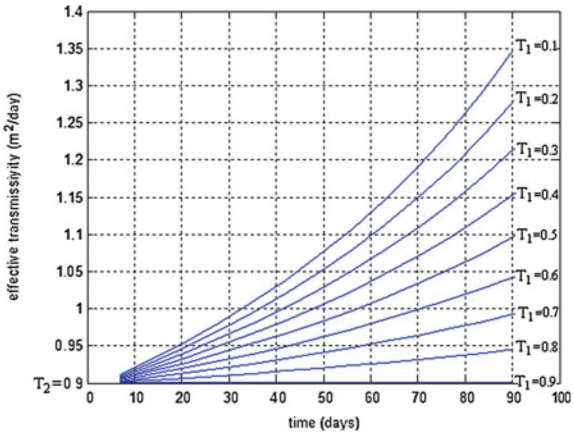

Fig. 9.6 Master curves for effective transmissivities for $T_2 > T_1$

parameters of homogeneous interpretation models. They are effective exactly in the same sense as the effective transmissivities in ours; that is, they have to reproduce the actual potential differences between two measuring electrodes, assuming the homogeneity of geological objects in terms of electrical resistivity. [Use of the geophysical master curves from electrical sounding, of both three-

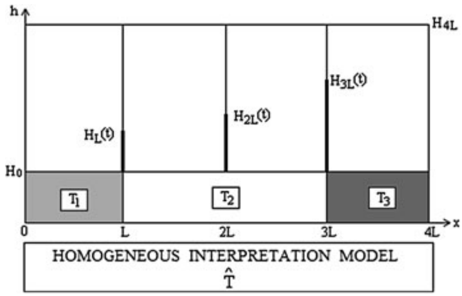

Fig. 9.7 Three-body confined aquifer and homogeneous interpretation model

electrode and dipole type, for interpreting pumping test data for corresponding combinations of not fully penetrating pumping, injecting, and observation wells in the steady-state regime was suggested by Gorokhovski and Jazvin (1970). At that time, pumping tests lasting from several days up to half of year had been common practice in the Soviet Union. I had used those master curves always when it seemed to be appropriate. However, I am not aware of somebody else who had been doing this].

Let us complicate the problem slightly. Namely, the hydrogeological process is the same as above with the same initial and boundary conditions but the hydrogeological object comprises three geological bodies (Fig. 9.7). The "observations," that is, the results of solving the forward problem, are obtained at $x = 2L$. The interpretation model is homogeneous. The flow within each geological body is described by three equations

$$\frac{\partial h(x,t)}{\partial t} = A_j \frac{\partial^2 h(x,t)}{\partial x^2} j = 1, 2, 3, \tag{9.43}$$

where x and t are the distance and time coordinates, and $h(x, t)$ is the hydraulic head in the intervals $[0, L]$ ($j = 1$), $[L, 3L]$ ($j = 2$), and $[3L, 4L]$ ($j = 3$). $A_j = T_j/S$ is the hydraulic diffusivity of body j, T_j is the hydraulic transmissivity of body j, and $S = 0.1$ is the storativity, which is the same for all bodies. The initial and boundary conditions are the following:

$$h(x, 0) = 0, \quad 0 \le x \le 4L, \tag{9.44}$$

$$h(0, t) = H_0 = 0 \text{ and } h(2L, t) = H_{4L} = 1\,\text{m}. \tag{9.45}$$

The inner boundary conditions on continuity of the hydraulic heads and the flux exist at $x = L$ and $x = 3L$:

$$\begin{aligned} &\lim_{x\to L}(h(L,t)) = \lim_{L\leftarrow x}(h(L,t)) \text{ and } T_1 \lim_{x\to L}\tfrac{\partial h(x,t)}{\partial x} = T_2 \lim_{L\leftarrow x}\tfrac{\partial h(x,t)}{\partial x} \\ &\lim_{x\to 3L}(h(3L,t)) = \lim_{3L\leftarrow x}(h(3L,t)) \text{ and } T_2 \lim_{x\to 3L}\tfrac{\partial h(x,t)}{\partial x} = T_3 \lim_{3L\leftarrow x}\tfrac{\partial h(x,t)}{\partial x} \end{aligned} \tag{9.46}$$

The explicit approximation of the hydraulic heads $h(2L,t_{i+1})$ can be presented as

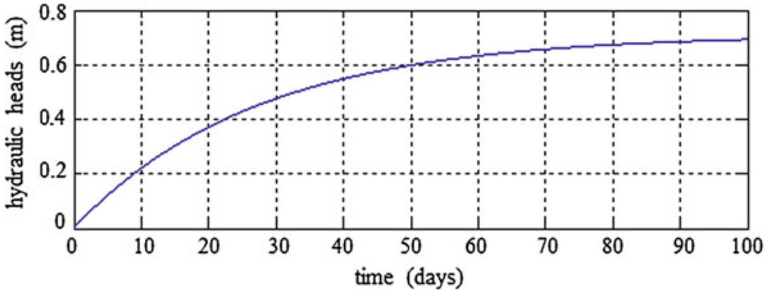

Fig. 9.8 Development of the hydraulic heads as $x = 2L$ during the first 100 days according to Eq. 9.49 ($T_1 = 0.1$, $T_2 = 0.2$, and $T_2 = 0.9$ m^2/day)

$$\frac{h_{i+1} - h_i}{\Delta t} = \frac{T_2}{S}\frac{h_{3L,i} - 2h_i + h_{L,i}}{L^2},$$

where $h_{\mathrm{i}} = h(2L, t_i)$, $h_{i+1} = h(2L, t_{i+1})$, $h_{L,i} = h(L, t_i)$ and $h_{L,i} = h(3L, t_i)$, or

$$h_{i+1} = h_i + \frac{T_2 \Delta t}{SL^2}(h_{3L,i} - 2h_i + h_{L,i}). \tag{9.47}$$

It follows from the inner boundary conditions (Eq. 9.46) that

$$h_{L,i} = \frac{T_2}{T_1 + T_2}h_i, \quad h_{3L,i} = \frac{T_3 + T_2 h_i}{T_2 + T_3} \tag{9.48}$$

Substituting the above results in Eq. 9.47 yields the following procedure for making up the "observations":

$$h_{i+1} = h_i + \frac{T_2 \Delta t}{SL^2}\left(\frac{T_3}{T_2 + T_3} + \left(\frac{T_2}{T_2 + T_3} + \frac{T_2}{T_1 + T_2} - 2\right)h_i\right). \tag{9.49}$$

The made-up "observations" for 100 days for the object with hydraulic conductivities $T_1 = 0.1$, $T_2 = 0.2$, and $T_2 = 0.9$ m^2/day calculated by Eq. 9.49 are presented in Fig. 9.8.

The effecting hydraulic transmissivity of the homogeneous model (Fig. 9.7) for the given structure of the geological object and the efficiency criterion ($\hat{h}_{i+1} = h_{i+1}$) can be calculated by the following equation, applying the implicit method this time:

$$\hat{T}_{i,i+1} = \frac{SL^2}{2(t_{i+1} - t_i)} \ln \frac{1 - 2h_i}{1 - 2h_{i+1}}. \tag{9.50}$$

Master curves in Fig. 9.9 are presented for the case when the hydraulic conductivities $T_1 = 0.1$ and $T_2 = 0.2$ m^2/day are fixed while the hydraulic conductivity T_3 varies. The same curves can be made up for other combinations of $T_{1\ldots3}$ and for objects with different numbers of geological bodies.

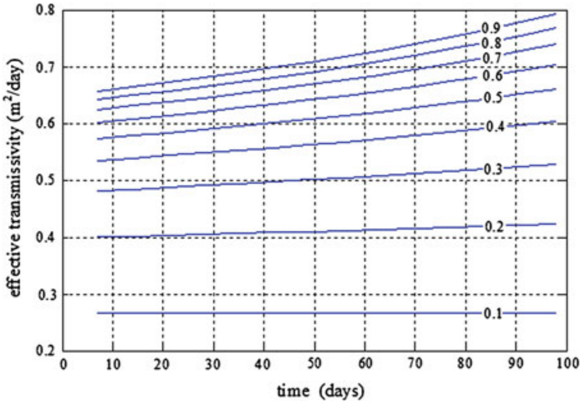

Fig. 9.9 Master curves obtained by applying the homogeneous interpretation model to the object presented in Fig. 9.8 with hydraulic transmissivities $T_1 = 0.1$ and $T_2 = 0.2$ m^2/day. Values of the transmissivities T_3 are shown on the pertinent plots

9.4 Conclusions

Often, transforming mechanisms can be applied to the formulation and solution of inverse problems related to underground flows. However, they cannot eliminate the inherent incorrectness of such problems. When manifolds of transforming mechanisms are created by the use of different weightings, the incorrectness is usually caused by the limited diversity of the weights assigned to the available observations. Whatever weights are applied, they act as if their values were in the interval [0, 1], or [−1, 1] if negative weights are applied. The failures can be caused also by unlucky choices of the models representing the real geological object and monitoring networks providing unsatisfactory amounts or diversity of data. Fortunately, the possibility of such failures can be identified before even starting the pertinent field investigations and taken into consideration in the stage of designing the pertinent projects. Projects can be corrected and optimized during their implementation based on incoming information. Thus, the approach based on transforming mechanisms permits the best (according to an accepted definition) results to be obtained. However, since our notions of geological objects are just models and, as such, false, the results of solving inverse problems are uncertain, meaning that it is impossible to evaluate their inaccuracy in a provable way.

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Chapter 10
Conclusion

Contemporary computational techniques permit simulation of any predictive problem based on up-to-date hydrogeological theories and concepts. The real issue is the reliability of the simulation results, their uncertainty. Geological objects and their properties are not known in full, and how the inaccuracy of a simulation model can affect the simulation results is unknown. Hornung (1990) writes: "One cannot substitute lack of theory and/or data by sophisticated mathematical models for parameter identification." In this sense, hydrogeology does not differ from other sciences: "Science is uncertain; the moment you make a proposition about a region of experience that you have not directly seen then you must be uncertain. But we always must make statements about the regions that we have not seen, or whole business is no use," as the great physicist and Nobel Prize winner Feynman (1965) wrote.

Hydrogeology is an applied science in the sense that we usually, if not always, "must make statements about the region we have not seen" and make decisions based on incomplete and erroneous data (US EPA 1987). Our best decisions are uncertain still and do not warrant success. Even a post audit demonstrating the failure or success of a decision does not mean that the decision was bad, or good. In the 1960s or 1970s, I read a book by an American author, I guess the author is Simon, about decision-making. One of his examples impressed me strongly. A person who needs to come to New York from San Francisco asks his friend whether it is better to fly or to go by car or train. The friend advises him to fly. The person flies. The airplane crashes. The person perishes. Thus, the post audit is disastrous, but does this mean that the advice and the person's decision to fly were bad? A successful post audit does not make the corresponding decision good either. Possibly, the same result could be achieved in more effective (economically or technologically) ways. Thus, we must judge the quality of our decisions based on the information available at the time of the decision-making.

In applied hydrogeology, the results, including the results of predictive modeling, are either a basis for decision-making or a goal per se. In both cases it

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*, SpringerBriefs in Earth Sciences, DOI: 10.1007/978-3-642-23722-5_10,

must provide the best results in some predefined sense with what we have (US EPA 1987). In my opinion, engineering experience, where it exists, seems to be the best practical tool for estimating probabilities of failure; for example, mass construction of family houses in geologically well-studied territories often makes geotechnical explorations unnecessary. Construction of small dams and reservoirs might also be based on simplified or reduced explorations. Practitioners know which models and model parameters are best to use for evaluating dam stability and water losses from reservoirs in given geological conditions. They may be wrong sometimes, and the rate of failed decisions can be interpreted as an approximation of the uncertainty.

But, what if the required experience does not exist? This usually happens in the case of unique projects where failures carry great financial or environmental risks. Contemporary computers and computational techniques permit the development of a surrogate for engineering experience, by applying simulation models based on geological considerations to fully known, different real worlds, i.e., to more complex models. (The certainly known details of the real worlds can and must be included in the two-level modeling). Comparing the results obtained from a simulation model (or several models) applied to numerous real worlds permits evaluation of how different factors could affect the simulation results for a given predictive problem. This is what I call two-level modeling. Essentially it is Monte Carlo simulation, only the other way around: the real worlds are changing, but the predictive model remains the same; only its effective parameters are changing, as demonstrated by the conceptual examples in Chaps. 5–8.

Since the factors affecting the "observations" in the real worlds are numerous and not all of them are taken into consideration in the simulation model(s), the issue arises of how to generalize the results of the simulation model calibrations on different real worlds in a practical, workable way. Transforming mechanisms, describing how the actual geological parameters convert into effective parameters of simulation models in an accepted formulation of the predictive problem, can be one approach to such generalization. The transforming mechanisms in the conceptual examples of Chaps. 6–8 clearly demonstrate that, in the case of dynamic processes such as underground water flow and mass transport, conversion of actual properties into effective parameters is not of statistical nature. The effective parameters are characteristics of the systems made up by geological conditions, structures of models, boundary conditions, criteria of effectiveness, monitoring networks, and time. The transforming mechanisms provide the effective parameters only for the systems in which they are obtained. Any changes of the systems lead to change in their transforming mechanisms. Thus, the transforming mechanisms and effective parameters for predicting water table or hydraulic heads may not be effective for evaluating streamlines or fluxes, and so on.

Transforming mechanisms, in particular their affecting factors, can be a tool for developing the methodology of field investigations. They demonstrate the importance of knowledge about the geological properties of different parts of the object for the accepted formulation of the predictive problem. They can be applied to formulate and solve inverse problems, or more accurately, to find actual parameters of more sophisticated models (objects) by applying less complex interpretation models as well (Chap. 9). The corresponding approach is similar to the approach to interpreting geophysical data, and in particular data from electric prospecting. Again the correctness or incorrectness of a given formulation of an inverse problem can be evaluated prior to starting field explorations.

It should be emphasized once more that transforming mechanisms and two-level modeling do not exclude the uncertainty of the simulation result. Also, I do not insist that the suggested approach is the only one possible, or the best for alleviating the issue of the uncertainty of hydrogeological simulation results. I hope that this work will help in the search for other, maybe quite different, ways to make hydrogeological modeling more informed and consequently better. Hydrogeology is a science, though partly an art also, and it must be treated as a science and use scientific methodology, which according to the great physicist and Noble Prize winner Bridgman (1955), "is nothing more than doing one's damnedest with one's mind, no holds barred."

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Afterword

Before coming to the United States in 1991, I worked for 35 years in applied geophysics, hydrogeology, geological engineering, and as a professor at two Universities in the Soviet Union. In this country I work for 20 years: with a private firm on projects ordered by Environmental Protection Agency (U.S. E.P.A.), as an instructor in a few colleges, a developer of models of underground flow and mass transport in the University of Georgia, where I received a Masters Degree in Applied Mathematics, and as a grantee with U.S. E.P.A. I think that comparison of my Soviet and American experiences may be of interest for readers.

At the very beginning of my professional career, I tried to apply statistical methods as much as I could to the results obtained by my colleagues and me. My colleagues were appreciative when I used such statistical methods as regression analysis, analysis of variances, discriminant analysis, and some others to their data especially when the data sets were huge. But they were usually skeptic about confident intervals and probabilities related to hypothesis testing, regressions, and so on. Their skepticism, based on their practical experience and common sense, made me reflect on the role of the statistical methods in geological applications. The results of my reflections are presented in Chap. 3. Briefly, although statistics is an effective tool for analysis of geological information, it is useless for provably evaluating the uncertainty of the simulation results in the case of modeling dynamic processes. In 1974, I wrote a pamphlet (Gorokhovski 1977) in which I considered this issue. Many colleagues were positive about my work in personal communications. A well-known geologist stopped speaking to me for 5 years. However, no positive or negative reviews appeared in professional publications. An American publisher bought the right to publish the pamphlet and I got my first $500. This made my wife Inna happy, as she could shop in ‘Berjozka’, where only people having foreign currency could shop, the privilege not available to most Soviet citizens. But the pamphlet was never published abroad.

I was already aware of the philosophical concept that all models are false and therefore it was impossible to prove the validity of modeling at that time. But we

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can reiterate about the uncertainty of the simulation results as much as we wish. The models remain our tool, likely our best one, for envisioning the effects induced by natural or man made impacts on geological surroundings. So in my opinion, the goal should be finding how to achieve the best with what we have, as US EPA (1987), states.

Once, while preparing simple problems for my students on evaluating effective parameters like those presented in Sect. 6.2, I found that some of the effective hydraulic conductivities obtained by the least squares method are negative. It was not the first time I saw physically incorrect results. Accordingly to the common practice, I discarded them based on the definition of incorrectness. But formally that definition assumes the absence of a mathematical solution. In the examples I was working with, the solutions in the mathematical sense existed. Due to the simplicity of the examples, I discovered some system and learned what geological structures are prone to obtaining the negative effective hydraulic conductivities. Then the question emerged as to what was incorrect in the problem formulation? The same well-conditioned system of equations yielded physically correct solutions with some combinations of the actual properties and incorrect ones with others. Thus the problem was correct mathematically. Two weeks of jogging and thinking led me to the concept described in Chap. 5.

I was happy with my finding, in particular with the properties of affecting factors. But the concept of the transforming mechanisms and their properties seemed so self-evident that I was concerned that somebody else would come to the same concept soon. To keep my priority, I wrote a paper (Gorokhovski 1982) and sent it in a paper repository. Such repositories in the Soviet Union did not require independent peer reviews and provided a very fast registration as a paper (3 months). Then the paper could be referred to as a publication (They also could be ordered and bought). Later the concept was published two more times (Gorokhovski 1986, 1991).

To my knowledge, the concept was original, absolutely new. Since the concept contradicted with the common notion, existing at present also, that the effective parameters of hydrogeological models are some statistics of the pertinent property values, the examples in my publications were such that they could be easily checked using a calculator or even by hand. But again, my colleagues demonstrated little interest in the concept. No response, positive or negative, appeared in the professional media, though in personal communications they called it interesting and promising (Sorry, I am not accurate. I had one negative response. A prominent Soviet hydrogeologist after reading my first paper on the transforming mechanism, Gorokhovski 1982, told me: “You are not modest”, and that was it. The reason for such severe judgment was the phrase ending Chap. 5 about the possibility of using the transforming mechanisms not only in hydrogeology but in other fields as well). So I decided that there was a need for a more detailed publication with more examples, maybe slightly more sophisticated, but transparent still.

At that time I worked as a docent (associate professor) of the Geology and Geography Department of the Rostov State University. My teaching load in the Spring semester of 1991 was 16 class hours a week, plus 10 course projects, plus

13 master thesis, plus consulting (I mention only my last semester with the University, because I remember it distinctly. But this load was close to average, if I was to exclude master theses which we did not have in the winter semesters). My desk was one of five in a shared office. A typewriter occupied the sixth one. We consulted students and performed all necessary jobs in this office. For a short time, a real PC was available to me but only for two hours per week. I was deprived even those hours very soon. Instead I got, in my full possession, a Soviet PC. The PC had a RAM of 64 Kb and a tape recorder instead of a hard drive. My graduate students used this PC for solving some simple problems related to their theses. I used it for preparing my lectures and other materials and for solving some problems related to teaching. In other words, there was no hope for me to develop my concept further in those circumstances.

In 1990 I met and befriended Dr. Zia Hosseinipour, an American scientist working on a project of cleaning up the low flow of the river Don. Returning to the United States, he asked me whether I would like to work there. My response was immediate: “Yes”. For me, as for most Soviet scientists, working in the United States was a dream. The American science, scientists and work conditions, including salaries, were a benchmark. I hoped also that I would be able to continue my work on the concept of the transforming mechanisms and some other projects.

In the spring of 1991, I got an invitation from an American firm to work on a project. To have an invitation for a job abroad was not enough for leaving the Soviet Union at that time. You needed your bosses’ consent. My University bosses did not want me to go. To make a long story short, being in complete despair, I took the liberty of calling Professor V.I. Sedletski. We were not friends. He was a head of the Mineralogy Chair of the department. More essential, he was a vice-president of the North Caucasus Science Center of Higher School. He told me that he needed a couple of days. Then I should start the process again. I got the desired permission to leave for the United States 4 days later. I owe the deepest gratitude to V. I. Sedletski still.

About 2 months later Zia Hosseinipour introduced me to Dr. James Martin, Head of the Athens, Georgia, branch of the company that hired me. Dr. Martin immediately took me to my office. My first American shock happened when I saw it: two desks, one with PC and the other with a telephone and a chair to travel between the desks. The office was mine only!

I started working, and nobody asked what I was doing during the first 3 months. It was absolutely different from my previous experience. In the Soviet Union, every supervisor asked you how your work was going, whether it was going accordingly to the planned schedule, and so on. And most annoyingly, it did not matter whether the supervisor understood or not what you were doing, the supervisor told you what to do and how to do it. So I was a little worried that Dr. Martin did not ask, teach, and advise me. Zia explained that James considered me as an expert in my field. When I finally finished my project, he would send it for review. In the meantime, if I had a problem, I should go to James and he would do everything he could to help me.

I got a problem when the project was almost finished. James passed me an instruction on conducting the sensitivity analysis. According to the instruction, I had to select the most important model parameters and to evaluate the model's sensitivity to each selected parameter, having fixed all others on their average levels. In my case, the block of the model describing mass transport through the vadose zone, contained 23 parameters when the zone was assumed homogeneous. How to decide which parameters are most important and on what average levels the not so important parameters should be fixed were not clear: the task was to validate the model in general without any specificities related to object structures and properties. Even if I selected the important parameters correctly and fixed all others on the right average levels, why would the sensitivity of a parameter obtained in such a way be representative? It can depend essentially on combining particular values of entire sets of the governing parameters. As I understand, the requirement or advice to fix all other parameters on their average level was dictated by the desire to make the sensitivity analysis workable. But there are other ways to make the sensitivity analysis workable, at least in my case. The most natural way is to perform the sensitivity analysis in the dimensionless form as I taught my Soviet students to do. My model was governed by three dimensionless parameters in the steady-state version and by four or five ones in the transient version. All these parameters are important. The sensitivity could be studied in the maximal realistic domain comprising all participating parameter values. The results for such a small number of the dimensionless parameters can be presented as contour maps. They can also be recalculated for any set of all actual parameter values. So I came to James and refused to do the sensitive analysis as the instruction required. He asked: “Why?” I explained. And, the second shock, his response was: “Well, do it as you consider the best”. In the Soviet Union, my boss would either tell me: “Do not pretend that you are the cleverest one. Do what you are told to do” or, if I were more fortunate, the boss would make me send a detailed letter to the instruction's authors and wait for their response.

I could say more positive words about the conditions under which research is being done in the United States. Sure there is control. But this control is not by the administration but usually by peers. They review your project, its implementation on different stages, and the final product. And you can dispute their conclusions if you disagree. The administration helps you, since you do the job (They are for you, not you for them). They also help you to get any information you wish (I found here the Russian text books on mathematics which had been used in Russian schools more than 60 or even 70 years ago. I could not find them in the Soviet Union).

However, not all my impressions related to scientific research in the U.S.A. are so positive. I was surprised by the standard approaches to the applied scientific researches by many of my American colleagues. The above instruction on the sensitivity analysis is just one example. It describes a standard procedure which does not take into consideration the specificity of the situation. The standards are useful and convenient. They save time and serve as a safeguard for engineers. But they do not have any relation to the real science and scientific research. Geological explorations deal with objects which are not known in full. In this sense they are scientific, and the best way to conduct them is “doing one’s damnedest with one’s mind” (Bridgman 1955). I taught my Soviet students that if they act as engineers, they have to follow the standards to cover themselves, even if they do not like or disagree with the standards. But if they work as researchers or scientists, the only limitation on their work is the detailed protocol of their actions and a clear presentation of their concepts and results. I rarely observed my American colleagues, realizing such a scientific approach, though the protocol for them seems to be about a holy thing.

Soviet hydrogeological models had bad interfaces in my time. This required that their users understood well the hydrogeological structure and properties of the object as well as the process they were simulating and its computational algorithm and were prepared to make non-trivial decisions sometimes. On the other hand, the American models are usually user friendly: their developers try to foresee and prevent any issue that a user could meet. And this is very convenient and effective, if the modeler is a professional. However, the convenience permits performing modeling by lay-modelers as well. The first American model, I worked with, led you through simulations, prompting what to do and even gave optional model parameters values if you had issues with their assigning. Once a colleague, who had a masters degree in Environmental Protection and worked with the same model, asked me to explain what the hydraulic conductivity is. In turn I was interested to know how she simulated her problems, having no notion of the hydraulic conductivity. She explained that she just followed prompts of the software while assigning different properties to different soils. I think that the example does not require any comment about the uncertainty of simulation results.

The above example leads me to compare the Soviet and American education systems. When we arrived at the United States, our American friend who was teaching Mathematics and Russian in a high school invited my wife to visit a lesson on Mathematics in his freshman year class. When I met my wife that evening, she was excited: the lesson started with repeating the table of multiplication. In the Soviet Union, we learned it in elementary school and never returned to it again. I even cannot imagine a student of the fifth grade not knowing the multiplication table in the Soviet Union.

I have taught precalculus in several colleges in this country. There was no such subject in Soviet Universities and Institutes in my time. All Soviet students were studying the same subjects and in the same details (Those who wanted to get some additional knowledge usually had the opportunity to do this). Students entering Universities and Institutes that required knowledge of algebra, geometry, and trigonometry had to pass entry tests. If they were not prepared properly, they failed.

The students in geology, hydrogeology, geological engineering, and geophysics of all Universities had the same syllabi (again, those who wanted to get some additional knowledge usually had the opportunity to do this). Any future geophysicist studied, besides geophysics and pertinent physics and mathematics, general geology and hydrogeology, paleontology, historical geology, mineralogy, tectonics, geology of the Soviet Union and so on, though in less detail compared to geologists and hydrogeologists. So it was expected that geophysicists were aware of hydraulic conductivity, geological age, and most other main geological notions and geologists and hydrogeologists have the knowledge on geophysics which permits understanding methodology and interpretation of geophysical explorations. Such education makes easier teamwork and even changing the fields of interest as it happened to me.

When I first met my American colleague in his University office, he was on the phone, explaining to somebody the method of characteristics. This was also some kind of surprise. I started recollecting how many Soviet hydrogeologists I knew, who were able to explain the method of characteristics: maybe, half a dozen not more. And here, the first one I met knew. I was delighted. But later I came to the understanding that many American hydrogeologists are rather mathematicians applying mathematics to hydrogeology. Hydrogeology is rather secondary for them, just a field for applied mathematics.

Returning to my first American model, it is defined as a screening level one. The model is not interesting per se. It comprises two blocks. The first one simulates the one-dimensional mass transport from a landfill through the vadose zone which could be piece-wise homogeneous. The second block simulates filtration within a homogeneous confined aquifer on the horizontal base. The flow in the aquifer is considered one-dimensional and steady state with constant and known seepage. No sorption, no degradation. The goal is to evaluate the arrival time for the contaminant from the landfill to an intake well which also works in a steady-state regime.

I was interested in the first block mostly. The block simulates input of the pollution in the confined aquifer which seems to me a little strange. Sensitivity analysis of the simulation results showed that for some physically acceptable values of the dimensionless parameters and the pertinent physical characteristics the contaminant mass coming into the confined aquifer were negative. Before writing my report, I informed the leader of the team working on developing the model about my discovery. He did not show any surprise and said that this problem was not a major one and would be corrected. I assume that he already knew about the problem.

I mention this story not to demonstrate that American modelers are bad. On the contrary, they are thorough professionals. Although the model I worked on had already been in practical applications , it was still in a stage of development . So errors could happen. The reason for me to tell this story came later when I was presenting my dimensionless sensitivity analysis at a conference. I concluded my presentation by saying that I discovered the negative concentration in the output of a block. We cannot expect that a modeler solving a practical problem has time and possibly skills for performing such thorough analysis. I suggested that every model which is to be used in practical applications must be tested and licensed by an independent body. The response of the audience was instant and unanimous: “No, this is not the American way”. My arguments that they go to licensed doctors and lawyers, who send their kids to licensed schools, and so on did not change the response of the colleagues: licensing the models developed by them is not the American way.

Let us return to my concept of the transforming mechanisms and two-level modeling. In 1993, I told a known American geostatistician that effective parameters of hydrogeological simulation models are not statistics and explained why. He answered that it was very interesting and that he liked my approach. Later, I sent him my paper (Gorokhovski 1996). His response was brief: “I like this less”. I never heard from him again. I gave my paper to another well-known geostatistician during the same conference. He promised to review the paper and to send his review to me. He did not. I asked him about his opinion on my paper when we met at another conference. He told me that he read it in the airplane on his way back from the previous conference, was very interested and was going to send me a review but could not find my paper. He asked mr to give him one more copy. I sent it immediately. I never heard from him again. I tried to publish several papers on my concept and made several presentations in the United States. Some of my papers were rejected (Interestingly, one review started with the phrase: “I do not understand what the author is about”. Well, if you do not understand, it would be reasonable to return the paper to the editor. But the reviewer continued with unmerciful critique of what he or she did not understand. When I asked the editor to pay attention to this fact, he responded that he trusted his reviewers). Anyway, a couple of papers and texts of my presentations were published. The response was the same as in the Soviet Union: no response. My conclusion was also the same: I have to describe the concept in a more detailed but still transparent form. To do this has taken a long time and arduous effort which I do not want to describe here. But if you read these lines, then I have fulfilled my goal. It would not be possible in Russia, and I am grateful to the United States of America for giving me this wonderful opportunity.

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